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PHONON MEDIATED ELECTRON-ELECTRON INTERACTION IN TWO-BAND SUPERCONDUCTORS

Bachelor's thesis

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Contents

1 Introduction **4**

1.1 Overview 4

1.2 Multiband superconductivity 5

1.3 Purpose and Organization of the Thesis 6

2 The Hamiltonian of the System **7**

2.1 The Full Hamiltonian and Second Quantization 7

2.2 Electronic Hamiltonian 8

2.3 Phonons 9

2.4 Electron-Phonon Interaction 9

3 Effective Electron-Electron Interaction **11**

3.1 Unitary Transformations in a Single Band Case 11

3.1.1 Fröhlich's Transformation 11

3.1.2 Wegner's transformation 11

3.2 Fröhlich's Transformation in a Multiband Setting 12

3.3 Effective Two-Band Electron-Electron Interaction 14

3.3.1 Limiting the Interaction to Shells in k-space 15

3.3.2 Intraband Coupling 17

3.3.3 Interband Non-FFLO Coupling 17

3.3.4 Interband FFLO Coupling 18

4 The Superconductive (Non-FFLO) Hamiltonian **20**

4.1 Mean-field Approximation 20

4.2 Diagonalization 21

4.2.1 Bogolyubov Transformations 21

4.2.2 Bogolyubov Transformation of the Mean-field Hamiltonian . . . 23

4.3 Gap Equations 25

5 Solutions to the Gap Equations in Special Cases **27**

5.1 Numerical Calculations 27

5.2 Only Intraband Pairing Electrons 28

5.3 Only Interband Pairing Electrons 30

5.4 Only Intra- or Interband Electron-Phonon Interaction 32

5.4.1 Repressed Intraband Interaction 32

5.4.2 Repressed Interband Interaction 34

6 Summary **36**

7 Acknowledgments **37**

References **38**

Foononite poolt vahendatav elektron-elektron interaktsioon kahetsoonilistes üli-juhtides **42**

1 Introduction

1.1 Overview

Superconductivity was discovered by H. Kamerlingh Onnes and his assistant G. Holst in the year 1911 in Leiden [1] when they observed that the resistivity of mercury suddenly vanishes if cooled below 4.2 K (the critical temperature, T_C). The existence of a critical current and magnetic field above which superconductivity is lost was identified shortly thereafter. In 1933 W. Meissner and R. Ochsenfeld showed that the magnetic field is expelled from superconducting samples, acting as perfect diamagnets. This is a fundamental property of superconductors which sets it apart from perfect conductivity.

Two years later F. and H. London [2] proposed a modification to Ohm's law (named the London equations) for the superconducting current carriers, which also described the Meissner effect and gave an expression for the magnetic field penetration depth (an important characteristic length). Based on the Landau's theory of second order phase transitions and gauge invariance, a phenomenological theory of superconductivity was proposed 15 years later by V. Ginzburg and L. Landau [3]. It was shown that (in the case of type II superconductors) the magnetic field can partially penetrate the sample by so-called vortices and form the Abrikosov lattice [4].

In 1950 H. Fröhlich [5] suggested that the origin of superconductivity could be the interaction between lattice vibrations (phonons) and electrons. The prediction of this hypothesis was the isotope effect: the mass of the ion has no effect on the material's electric properties, but it does alter the phonon frequencies. This has been confirmed in monoatomic crystals. In 1957 the first *microscopic* theory of superconductivity was put forth by J. Bardeen, L. Cooper and J. Schieffer (BCS) [6, 7], describing superconductivity as a macroscopic quantum phenomenon. It relied on the existence of Cooper pairs [8]: electrons near the Fermi surface with opposite momenta form a stable pair however small (but attractive) their interaction. These form a highly correlated condensate with an energy gap 2Δ centered on the Fermi level which is the energy needed to break up a Cooper pair into two free electrons. The BCS theory made several predictions and was found to be in a very good agreement with experiment (quite surprising to many, considering the simplicity of the model). Bogolyubov derived the theory by a canonical transformation of the electron-phonon Hamiltonian[9] (the method which shall be used in this text) and Gor'kov [10] showed that the Ginzburg-Landau theory can be derived from the BCS theory near T_C with Δ proportional to the phenomenological order parameter.

For a long time $T_C \approx 23.3\,\mathrm{K}$ of Nb_3Ge was the highest known critical temperature. It was accepted as the practical maximum because the parameters determining it in the BCS theory (for example the phonon spectrum) could not be varied much more in real mate-

rials. So the accidental discovery of high-temperature superconductivity in a lanthanum-based cuprate perovskite in 1986 by Bednorz and Müller [11] (for which they received the Nobel Prize in Physics just after a year) was shocking to the scientific community. In a few years many new superconducting materials were discovered, some with a T_C above the boiling point of nitrogen ($YBa_2Cu_3O_7$ (YBCO) was the first such material with $T_C \approx 90\,\mathrm{K}$), which made various applications practical like superconducting electromagnets (used in MRI/NMR, mass spectrometers, and particle accelerators) and sensitive magnetometers (Josephson junctions - two superconductors connected by a weak link). The theoretical work also intensified as scientists rushed to extend or find an alternative to BCS theory with antiferromagnetic spin fluctuations [12] and multi-orbital mechanisms among the many proposed. Despite that, now, almost 30 years after, a fully satisfying explanation has not been formed due to the complexity of the systems (related to the layer structure of the materials) which is itself now believed to be the cause of high-T_C superconductivity [13]. The higher T_C materials have more components, but superconductivity seems to require very specific doping ratios. This sets a limit to testing all different materials for superconductivity: MgB_2 for example, only a two-component system, was found superconducting below 39 K relatively recently in 2001, the highest known $T_C = 139\,\mathrm{K}$ is found in a six-component cuprate. A better theoretical understanding would aid in the search for new superconductors and it is a good testing ground for theoretical concepts which could be used in the context of other condensed matter systems. A good overview about the theory of high-temperature superconductivity is given in the freely available book by Mourachkine [14].

1.2 Multiband superconductivity

The present work is dedicated to superconductivity arising from electron-phonon interaction in a multiband setting. The BCS-theory (which has its origin in electron-phonon interaction) has been immensely successful and since newly discovered superconducting materials exhibit complex band structure [15], this is an obvious direction for advancement.

Early work has been largely concentrated on electron pairs formed inside the bands with the possibility for the pair to transfer from one band to the other (it was considered already in 1959 [16, 17] and has received interest recently as a possible mechanism for superconductivity in cuprates [18]). Whereas single band BCS superconductivity requires the interaction to be attractive, introducing pair transfer interactions can alleviate that condition. Kondo showed in 1963 that, even if the electron-electron interaction in one band is repulsive, the transition of pairs from one band to the other leads to higher critical temperature than if the bands are treated separately as in the BCS model [19]. There is

also the possibility of interband pairing[1] [20, 21, 22, 23] which is very often ignored. Modern theoretical models include extensions to the Ginzburg-Landau theory, Eliashberg theory (for strong coupling) and extensions to the BCS Hamiltonian (for weak coupling). A recent overview of them is provided here [24].

The effects of multiband superconductivity can be observed in a multitude of experiments including thermal conductivity [25] the critical field strengths and temperatures, characteristic lengths, energetic gaps and specific heat, as outlined by [24]. One of the difficulties lies in distinguishing multiband and anisotropic effects, as the differences can be subtle.

The most recognized multiband superconductor is MgB_2 the discovery of which in 2001 is largely responsible for the increased research in this area in the last decade. Other materials in which multiband effects are thought to be important are for example iron pnictides, cuprates and borocarbides (a recent overview is given here [24]). New superconductors with very different properties are still frequently discovered, but a unifying theory to explain them remains elusive.

1.3 Purpose and Organization of the Thesis

The aim of the thesis is to derive the complete set of effective electron-electron interactions for a two-band metal mediated by virtual phonons where the intraband as well as interband electron-phonon channels have been taken into account. The efficiencies of these electron-electron processes to induce superconductivity will be analyzed. In some particular cases the corresponding superconducting orderings will be considered in more detail.

The main body of the thesis is structured into four parts. The Hamiltonian of the system is set up in part 2. The Fröhlich's transformation is used to obtain the effective electron-electron interaction potentials in part 3. In part 4 the mean-field approximation is used and the Hamiltonian diagonalized. The spectrum of elementary exitations together with gap equations are obtained. Special cases, where some of the interaction potentials disappear, are considered in part 5. The concluding remarks follow.

All the calculations were performed by the author unless stated otherwise.

[1] The terminology is slightly confusing. *Interband superconductors* refer to the case where Cooper pairs formed inside bands can scatter to different bands. *Interband pairing* refers to the mechanism in superconductors where the electrons of a Cooper pair themselves can be in different bands.

2 The Hamiltonian of the System

2.1 The Full Hamiltonian and Second Quantization

The Hamiltonian is taken to be

$$
\begin{aligned}
H &= H_0 + H_{\text{el-ph}}, && (2.1)\\
H_0 &= H_{\text{el}} + H_{\text{ph}}, && (2.2)\\
H_{\text{el}} &= \sum_{\alpha,\mathbf{k},\sigma} \left[\varepsilon_\alpha(\mathbf{k}) - \varepsilon_F\right] a^\dagger_{\mathbf{k}\alpha\sigma} a_{\mathbf{k}\alpha\sigma}, && (2.3)\\
H_{\text{ph}} &= \sum_{j,\mathbf{q}} \hbar\omega_{\text{j}}(\mathbf{q}) \left(b^\dagger_{\mathbf{q}j} b_{\mathbf{q}j} + \frac{1}{2}\right), && (2.4)\\
H_{\text{el-ph}} &= \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\alpha_1,\alpha_2} \sum_{\sigma,j} G^j_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^\dagger_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} \left(b^\dagger_{\mathbf{k}_1-\mathbf{k}_2,j} + b_{\mathbf{k}_2-\mathbf{k}_1,j}\right), && (2.5)
\end{aligned}
$$

where $H_{\text{el}} + H_{\text{ph}}$ is the non-interacting part and $H_{\text{el-ph}}$ describes the interaction between electrons and phonons. The various symbols occurring in the Hamiltonian and described in detail in the following sections are:

$\hbar$ - Planck's angular constant

$a_{\mathbf{k}\alpha\sigma}$, $a^\dagger_{\mathbf{k}\alpha\sigma}$ - the annihilation and creation operators for an electron in band α with wavevector $\mathbf{k}$[2] and spin $\sigma \in \{\uparrow,\downarrow\}$

$b_{\mathbf{q}j}$ $b^\dagger_{\mathbf{q}j}$ - the annihilation and creation operators for a phonon in branch j with wavevector $\mathbf{q} = \mathbf{k}_2 - \mathbf{k}_1$

$\varepsilon_\alpha(\mathbf{k})$ - band α of the electronic spectrum

$\omega_{\text{j}}(\mathbf{q})$ - the jth branch of the phononic spectrum

$G^j_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2}$ - the electron-phonon interaction constants

Describing a many-body system via a Hamiltonian like (2.1) to (2.5) is very common in condensed matter theory and detailed derivation with examples can be found as introductory parts of many books on field theoretical approach to many-body physics. For example [26] and [27] were very useful in learning this method which is commonly known as the language of second quantization. Those books are also largely the basis for the next three sections.

This representation involves ladder operators which either add or remove particles to a state and allows to express the Hamiltonian directly in terms of possible processes

[2] Here and below bold typeface is used for vector quantities.

between particles which simplifies the interpretation. Additionally, no reference to the actual states (wave vectors) is necessary, all the information is contained in the Hamiltonian and the properties of the operators.

The combination $c^\dagger c$ is called a number operator (if c is an annihilation operator) and its eigenvalue gives the number of particles or exitations associated with an eigenvector. If the Hamiltonian of a system is expressed as $H = \sum_\mu E_\mu c_\mu^\dagger c_\mu$, then E_μ are the energies of the respective exitations.

Other combinations can be used to represent interactions. Scattering of a particle from state ν to μ can be described by the operator $c_\mu^\dagger c_\nu$ so $c_{\mu_2}^\dagger c_{\mu_1}^\dagger c_{\nu_2} c_{\nu_1}$ gives the first order interaction term. The scattering process can also involve a creation or annihilation of another particle like in (2.5).

2.2 Electronic Hamiltonian

The electronic Hamiltonian (2.3) describes a system of non-interacting Bloch electrons with wavefunctions $\psi_{\alpha\mathbf{k}\sigma}(\mathbf{r}) = u_{\alpha\mathbf{k}}(\mathbf{r})\, e^{i\mathbf{kr}}\chi_\sigma$ where $\mathbf{k}$ is in the first Brillouin zone, $u_{\alpha\mathbf{k}}(\mathbf{r}) = u_{\alpha\mathbf{k}}(\mathbf{r}+\mathbf{R})$, $\mathbf{R}$ is any lattice vector, and χ_σ is the spin part of the wavefunction. The energies with respect to the Fermi level are taken into account. In the jellium model for example, where the lattice potential is taken to be uniform (the phononic part reintroduces the interaction, but in a better way), the electronic Hamiltonian is shown to be

$$H_{\text{el}-\text{jellium}} = \sum_{\alpha,\mathbf{k},\sigma} \left[\frac{\hbar^2 \mathbf{k}^2}{2m_\alpha} - \varepsilon_F \right] a_{\mathbf{k}\alpha\sigma}^\dagger a_{\mathbf{k}\alpha\sigma}, \tag{2.6}$$

where m_α is the effective mass of the electrons in band α.

Dividing the electrons into bands is an approximation of the fact that electrons can occupy different orbitals which can hybridize in different ways. The a-operators actually describe quasiparticles which act like non-interacting electrons with different energy spectra.

Electrons are fermions (the Pauli exclusion principle applies) and so the creation and annihilation operators obey the Fermi anticommutation rules

$$\left\{ a_{\mathbf{k}_1\alpha_1\sigma_1}, a_{\mathbf{k}_2\alpha_2\sigma_2}^\dagger \right\} = \delta_{\mathbf{k}_1,\mathbf{k}_2}\delta_{\alpha_1,\alpha_2}\delta_{\sigma_1,\sigma_2}, \tag{2.7}$$

$$\left\{ a_{\mathbf{k}_1\alpha_1\sigma_1}, a_{\mathbf{k}_2\alpha_2\sigma_2} \right\} = \left\{ a_{\mathbf{k}_1\alpha_1\sigma_1}^\dagger, a_{\mathbf{k}_2\alpha_2\sigma_2}^\dagger \right\} = 0. \tag{2.8}$$

This means the wavefunction is antisymmetric under the exchange of electrons. These rules define the algebra of the operators and are thus used extensively in the following

sections.

Operators of the type $a^\dagger_\mu a_\nu$ $\mu \neq \nu$ do not appear in the Hamiltonian (2.1) which means that the system is operating in the clean limit (no impurity scattering) without any external fields.

2.3 Phonons

Phonons are lattice vibrations described with the Hamiltonian (2.4), so they act as independent harmonic oscillators. The wavevectors $\mathbf{q}$ can, as $\mathbf{k}$ in section 2.2, take values from the first Brillouin zone allowed by the periodic boundary conditions. The summation is over all the phonon branches. There are, in general, d acoustic branches and $d\,(m-1)$ optical ones, where d is the dimension of the crystal and m is the number of atoms in the primitive cell. For acoustic phonons the Debye frequency characterizes the maximum energy $\hbar\omega_\mathrm{D}$ of the allowed phonon modes. The Debye temperature is defined from $\hbar\omega_\mathrm{D} = k_\mathrm{B} T_\mathrm{D}$ and has a value from 200 K to 2000 K in metals which corresponds to 10 meV to 100 meV.

In contrast to electrons, phonons are bosons, and therefore adhere to the Bose commutation rules

$$\left[b_{\mathbf{q}_1 j_1}, b^\dagger_{\mathbf{q}_2 j_2}\right] = \delta_{\mathbf{q}_1\mathbf{q}_2}\delta_{j_1 j_2}, \tag{2.9}$$

$$\left[b_{\mathbf{q}_1 j_1}, b_{\mathbf{q}_2 j_2}\right] = \left[b^\dagger_{\mathbf{q}_2 j_2}, b^\dagger_{\mathbf{q}_1 j_1}\right] = 0, \tag{2.10}$$

which means that the wavefunction is symmetric under the exchange of phonons.

2.4 Electron-Phonon Interaction

The interaction between phonons and electrons is described by the Hamiltonian (2.5). Operators $a^\dagger_\mu a_\nu b^\dagger_\rho$ describe a process where an electron scatters from state ν to μ while emitting a phonon in state ρ and operators $a^\dagger_\mu a_\nu b_\rho$ describe the the same process while absorbing a phonon. The phonon and electron states are related by momentum conservation but are otherwise independent (they commute).

The G coefficients have an intrinsic symmetry which comes from the Hermiticity of the Hamiltonian. Let the Hamiltonian (2.5) be originally be given in terms of coefficients with no symmetries $\tilde{G}$. The Hermitian conjugate of that Hamiltonian gives

$$H^\dagger_{\mathrm{el-ph}} = \sum_{\mathbf{k}_1,\mathbf{k}_2}\sum_{\alpha_1,\alpha_2}\sum_{\sigma,j} \tilde{G}^{j*}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^\dagger_{\mathbf{k}_1\alpha_1\sigma} a_{\mathbf{k}_2\alpha_2\sigma}\left(b_{\mathbf{k}_1-\mathbf{k}_2,j} + b^\dagger_{\mathbf{k}_2-\mathbf{k}_1,j}\right). \tag{2.11}$$

As the sums over $\mathbf{k}_1$,$\mathbf{k}_2$ and σ_1,σ_2 are over the same vectors and bands, this can be written

as

$$H_{\text{el}-\text{ph}}^{\dagger} = \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\alpha_1,\alpha_2} \sum_{\sigma,j} \tilde{G}^{j*}_{\alpha_2\mathbf{k}_2,\alpha_1\mathbf{k}_1} a^{\dagger}_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} \left(b^{\dagger}_{\mathbf{k}_1-\mathbf{k}_2,j} + b_{\mathbf{k}_2-\mathbf{k}_1,j} \right). \tag{2.12}$$

Since the Hamiltonian is Hermitian, it can be written

$$\begin{aligned} H_{\text{el}-\text{ph}} &= \frac{H_{\text{el}-\text{ph}} + H^{\dagger}_{\text{el}-\text{ph}}}{2} && (2.13) \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\alpha_1,\alpha_2} \sum_{\sigma,j} G^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^{\dagger}_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} \left(b^{\dagger}_{\mathbf{k}_1-\mathbf{k}_2,j} + b_{\mathbf{k}_2-\mathbf{k}_1,j} \right), && (2.14) \\ G^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} &= \frac{G^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} + \tilde{G}^{j*}_{\alpha_2\mathbf{k}_2,\alpha_1\mathbf{k}_1}}{2} = G^{j*}_{\alpha_2\mathbf{k}_2,\alpha_1\mathbf{k}_1}. && (2.15) \end{aligned}$$

This is a general symmetry stemming from the Hermiticity and the form of the Hamiltonian. Similar arguments show that $\varepsilon_{\alpha}(\mathbf{k})$ and $\omega_j(\mathbf{k})$ are real.

3 Effective Electron-Electron Interaction

3.1 Unitary Transformations in a Single Band Case

3.1.1 Fröhlich's Transformation

In BCS theory, an effective (attractive) electron-electron interaction is introduced. Fröhlich showed [28], that this kind of interaction can have its origin in electron-phonon interaction. By performing a unitary transformation which eliminates the electron-phonon interaction an effective electron-electron interaction (and terms involving multiple phonons which are left out by perturbative considerations) is obtained.

Fröhlich's transformation is of the form

$$\tilde{H} = e^{-iS} H e^{iS} \tag{3.1}$$

with S a Hermitian operator chosen to mimic the interaction term (2.5) with the condition that it eliminates operators involving a single phonon operator.

The hermiticity of S guarantees that the transformation is unitary ($U^{\dagger}U = I$). A unitary transformation is essentially a rotation of the system in Hilbert space which preserves the inner product and thus all the calculated probabilities and averages of observables. An example of other unitary transformations is the time evolution operator.

The effective electron-electron interaction constants obtained this way for one band are

$$V_F(\mathbf{k},\mathbf{q}) = -\frac{|G(\mathbf{q})|^2}{[\omega(\mathbf{q})]^2 - [\varepsilon(\mathbf{k}+\mathbf{q}) - \varepsilon(\mathbf{k})]^2}. \tag{3.2}$$

Fröhlich's transformation does have a few problems. The most striking is the singularity in (3.2), which is in no way physical. Another problem is that S in (3.1) is not always easy to choose and needs to be basically guessed (this applies to general problems, here the known one band electron-phonon case is just generalized which is quite straightforward).

3.1.2 Wegner's transformation

A more advanced approach is to use the Wegner's transformation (also called the flow equations because the transformation is continuous) proposed relatively recently in 1993 and 1994 independently by Glazek and Wilson [29, 30] and Wegner [31] though in different contexts: the former in light-front chromodynamics and the latter in condensed matter physics which is more relevant here (it also shows the method's general applicability). A comprehensive treatment of the mathematical structure with an overview of the applications is given in [32].

Very generally, the differential equation to diagonalize a Hermitan matrix $H_0 = H(0)$ is the following

$$\dot{H} = [[N,H],H], \tag{3.3}$$

where N is a fixed diagonal matrix and $H(\infty)$ is diagonal and the off-diagonal elements decrease monotonically to zero. The differential equation for the corresponding unitary (at each point $Q^\dagger Q = 1$) transformation is

$$\dot{Q} = Q\left[Q^\dagger H_0 Q, N\right], \tag{3.4}$$

$$H = Q^\dagger H_0 Q. \tag{3.5}$$

Wegner's original transformation is obtained by letting $N = \mathrm{diag}(H)$ (not fixed), which represents the steepest flow toward the diagonal form of H_0. Applying it to the single band Hamiltonian yields an effective electron-electron interaction constants

$$V_W(\mathbf{k},\mathbf{q}) = -\frac{|G(\mathbf{q})|^2}{[\omega(\mathbf{q})]^2 + [\varepsilon(\mathbf{k}+\mathbf{q}) - \varepsilon(\mathbf{k})]^2}.$$

These are remarkably similar to Fröhlich's solution, only the sign is different, which consequently removes the singularities present in (3.2). It should also be noted that $V_W(0,\mathbf{q}) = V_F(0,\mathbf{q})$ and since this value is used for approximating the potential in BCS theory, it doesn't actually change anything.

Fröhlich's transformation is used in the following multiband case, but it remains an open problem whether the Wegner's transformation in a multiband setting would also give the same values as Fröhlich's with just a sign change. [3]

3.2 Fröhlich's Transformation in a Multiband Setting

If multiple bands are present, the transformation can still be carried out in essentially the same way as the original Fröhlich's (3.1) one with added band indices.

$$\tilde{H} = e^{-iS} H e^{iS} \tag{3.6}$$

with S chosen like this:

$$S = s + s^\dagger \tag{3.7}$$

$$s = \sum_{\mathbf{k}_1,\mathbf{k}_2} \sum_{\alpha_1,\alpha_2} \sum_{\sigma,j} \lambda^j_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} G^j_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^\dagger_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} b_{\mathbf{k}_2-\mathbf{k}_1,j}, \tag{3.8}$$

[3] It may be that introducing different bands will give some interference (off-diagonal) terms to the flow equations so the number of equations would increase but they could be coupled in a non-trivial way.

It is obviously Hermitian and the transformation unitary. Expanding the transformation and (keeping here and below only terms up to second order in G) gives

$$\tilde{H} \approx H + i[H,S] - \frac{1}{2}[[H,S],S] \tag{3.9}$$

$$\approx H_0 + H_{\text{el-ph}} + i[H_0,S] + i\left[H_{\text{el-ph}},S\right] - \frac{1}{2}[[H_0,S],S] - \frac{1}{2}\left[\left[H_{\text{el-ph}},S\right],S\right]. \tag{3.10}$$

λ is chosen so that electron-phonon interaction in first order is removed, which is achieved with

$$H_{\text{el-ph}} + i[H_0,S] = 0. \tag{3.11}$$

Using equations (2.2) to (2.5) and also the commutation rules for Fermi and Bose operators, this condition can be rewritten as[4] (the calculation is straightforward)

$$0 = \sum_{\mathbf{k}_1,\mathbf{k}_2}\sum_{\alpha_1,\alpha_2}\sum_{\sigma,j}\left\{\left\{1 + i\lambda^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2}\left[\varepsilon_{\alpha_2}(\mathbf{k}_2) - \varepsilon_{\alpha_1}(\mathbf{k}_1) - \hbar\omega_{\text{j}}(\mathbf{k}_2 - \mathbf{k}_1)\right]\right\}\right.$$
$$\left. \times\, G^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^{\dagger}_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} b_{\mathbf{k}_2-\mathbf{k}_1,j}\left(h_{\text{el-ph}} + i[H_0,s]\right)^{\dagger}\right\}. \tag{3.14}$$

This can be met if the expressions in the inner curly brackets are taken to be zero. This gives a value for λ:

$$\lambda^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} = \frac{i}{\varepsilon_{\alpha_2}(\mathbf{k}_2) - \varepsilon_{\alpha_1}(\mathbf{k}_1) - \hbar\omega_{\text{j}}(\mathbf{k}_2 - \mathbf{k}_1)} \tag{3.15}$$

and the transformed Hamiltonian becomes (by applying (3.11) to (3.10))

$$\tilde{H} = H_0 + i\left[H_{\text{el-ph}},S\right] - \frac{1}{2}[[H_0,S],S] - \frac{1}{2}\left[\left[H_{\text{el-ph}},S\right],S\right]. \tag{3.16}$$

The multiphonon interactions are left out. After somewhat lengthy rearrangements, the Hamiltonian with coefficients symmetrized with regards to Hermitian conjugation and Fermi commutation rules, is

$$H = H_{\text{el}} + H_{\text{el-el}}, \tag{3.17}$$

$$H_{\text{el}} = \sum_{\alpha,\mathbf{k},\sigma}\left[\varepsilon_{\alpha}(\mathbf{k}) - \varepsilon_F\right] a^{\dagger}_{\mathbf{k}\alpha\sigma} a_{\mathbf{k}\alpha\sigma}, \tag{3.18}$$

$$H_{\text{el-el}} = \sum_{\mathbf{K},\mathbf{k}}\sum_{\alpha_1,\alpha_2}\sum_{\alpha_1',\alpha_2'}\sum_{\sigma,\sigma'}\sum_{\mathbf{q},j} V^{j\alpha_1'\alpha_2'}_{\alpha_1\alpha_2}(\mathbf{K},\mathbf{k},\mathbf{q})\, a^{\dagger}_{\mathbf{K}+\mathbf{k}+\mathbf{q},\alpha_1'\sigma} a^{\dagger}_{\mathbf{K}-\mathbf{k}-\mathbf{q},\alpha_2'\sigma'} a_{\mathbf{K}-\mathbf{k},\alpha_2\sigma'} a_{\mathbf{K}+\mathbf{k},\alpha_1\sigma}, \tag{3.19}$$

[4] $h_{\text{el-hp}}$ is used for convenience:

$$h_{\text{el-ph}} = \sum_{\mathbf{k}_1,\mathbf{k}_2}\sum_{\alpha_1,\alpha_2}\sum_{\sigma,j} G^{j}_{\alpha_1\mathbf{k}_1,\alpha_2\mathbf{k}_2} a^{\dagger}_{\mathbf{k}_2\alpha_2\sigma} a_{\mathbf{k}_1\alpha_1\sigma} b_{\mathbf{k}_2-\mathbf{k}_1,j}, \tag{3.12}$$

$$H_{\text{el-ph}} = h_{\text{el-ph}} + h^{\dagger}_{\text{el-ph}}. \tag{3.13}$$

$$V^{j\alpha_1'\alpha_2'}_{\alpha_1\alpha_2}\left(\frac{\mathbf{k}_1+\mathbf{k}_2}{2},\frac{\mathbf{k}_1-\mathbf{k}_2}{2},\mathbf{q}\right) = \frac{1}{2}G^{j}_{\alpha_2\mathbf{k}_2,\alpha_2',\mathbf{k}_2-\mathbf{q}}G^{j*}_{\alpha_1',\mathbf{k}_1+\mathbf{q},\alpha_1\mathbf{k}_1}$$

$$\times \left[\frac{\hbar\omega_\mathrm{j}(\mathbf{q})}{\left[\varepsilon_{\alpha_2'}(\mathbf{k}_2-\mathbf{q})-\varepsilon_{\alpha_2}(\mathbf{k}_2)\right]^2-\left[\hbar\omega_\mathrm{j}(\mathbf{q})\right]^2}+\right. \tag{3.20}$$

$$\left.+\frac{\hbar\omega_\mathrm{j}(\mathbf{q})}{\left[\varepsilon_{\alpha_1'}(\mathbf{k}_1+\mathbf{q})-\varepsilon_{\alpha_1}(\mathbf{k}_1)\right]^2-\left[\hbar\omega_\mathrm{j}(\mathbf{q})\right]^2}\right], \tag{3.21}$$

where the center of mass momentum (or wave-vector) $\mathbf{K}=\frac{\mathbf{k}_1+\mathbf{k}_2}{2}$ and the momentum of the first electron in center of mass frame $\mathbf{k}=\frac{\mathbf{k}_1-\mathbf{k}_2}{2}$ are introduced for convenience. The electron-electron interaction coefficients have the following symmetries:

$$V^{j\alpha_1'\alpha_2'}_{\alpha_1\alpha_2}(\mathbf{K},\mathbf{k},\mathbf{q}) = V^{j\alpha_1\alpha_2*}_{\alpha_1'\alpha_2'}(\mathbf{K},\mathbf{k}+\mathbf{q},-\mathbf{q}), \tag{3.22}$$

$$V^{j\alpha_1'\alpha_2'}_{\alpha_1\alpha_2}(\mathbf{K},\mathbf{k},\mathbf{q}) = V^{j\alpha_2'\alpha_1'}_{\alpha_2\alpha_1}(\mathbf{K},-\mathbf{k},-\mathbf{q}). \tag{3.23}$$

This concludes the transformation.

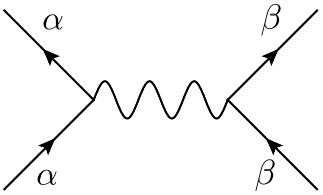
3.3 Effective Two-Band Electron-Electron Interaction

From here on, only two bands will be looked at. That means 4 kinds of processes remain. $\alpha\neq\beta$ denote the bands in figures 3.1a to 3.1 and it should be kept in mind that the spins do not change in the interaction.

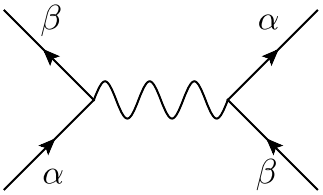
(a) Intraband pair-transfer processes

(b) Interband pair-transfer processes

Figure 3.1: Processes involving intraband pairs

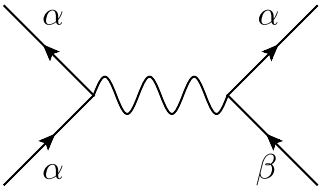


(a) With band switching

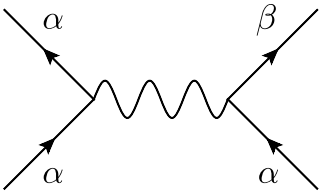


(b) Without band switching

Figure 3.2: Interband pair scattering processes



(a) Interband to intraband



(b) Intraband to interband

Figure 3.3: Pair transformation processes

Furthermore, only singlet pairs will be considered, so $\sigma' = \overline{\sigma}$ [5] in 3.19. Also, only the effect of one phonon branch shall be taken into account, so the index j will not be written. This has no qualitative effects, since it only appears in the interaction potential and those are eventually taken to be constants.

3.3.1 Limiting the Interaction to Shells in k-space

Not all possible interactions are considered. First of all, the potential (3.20) is divergent at some points so it needs to be approximated. Secondly, in order to diagonalize the mean-field Hamiltonian in section 4.2, it is imperative that not all different products of a-operators appear. The problem would still be diagonalizable, but a matrix of the order of different states would have to be diagonalized. Clever restriction of the states can and will lead to this matrix being block-diagonal and the those blocks can be diagonalized separately.

The most obvious choice is to restrict all the interacting electrons to be close to the Fermi level. The same thing is done by BCS and it is highly motivated for heavy fermion systems [33]. It is also is motivated by phonon statistics, which implies

$$\hbar\omega(\mathbf{q}) < \hbar\omega_{\mathrm{D}} \ll \varepsilon_F \tag{3.24}$$

[5] Here and below a slightly unconventional style of notation is used: $\overline{\uparrow} = \downarrow$ and $\overline{\downarrow} = \uparrow$. Usually the reversing of spin index is denoted with a minus, but this makes the equations less

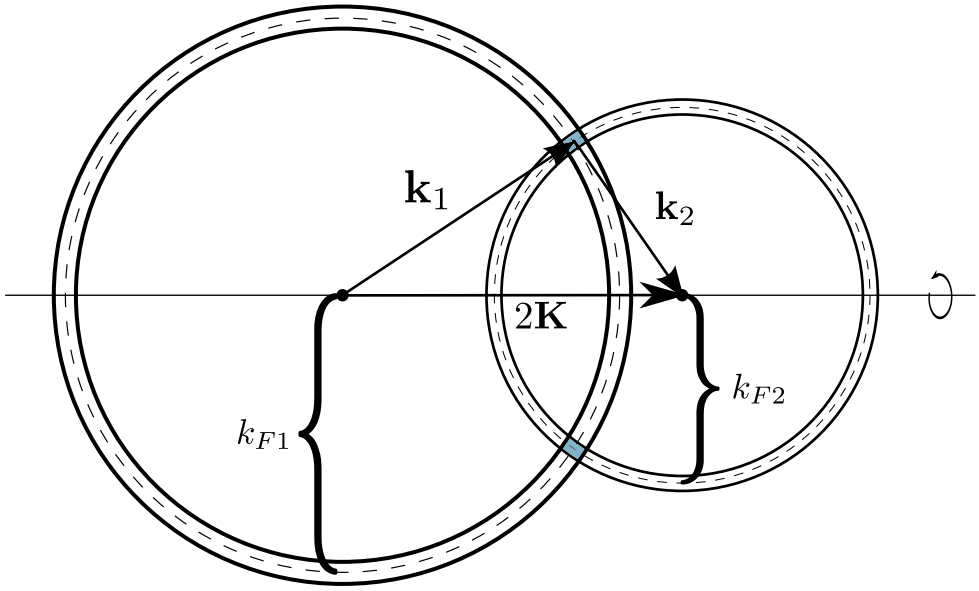


Figure 3.4: Fermi spheres of the interacting electrons

and this in turn allows one to make an approximation whereby electronic states with energy below $\varepsilon_F - \hbar\omega_{\mathrm{D}}$ are all occupied and above $\varepsilon_F + \hbar\omega_{\mathrm{D}}$ unoccupied. This determines a definite volume in k-space which is a spherical shell when $\varepsilon(\mathbf{k}) = \varepsilon(|\mathbf{k}|)$.

In a two-band case, the picture is a little bit more complicated since

$$\varepsilon_F - \hbar\omega_{\mathrm{D}} < \varepsilon_1(\mathbf{k}) < \varepsilon_F + \hbar\omega_{\mathrm{D}} \tag{3.25}$$

and

$$\varepsilon_F - \hbar\omega_{\mathrm{D}} < \varepsilon_2(\mathbf{k}) < \varepsilon_F + \hbar\omega_{\mathrm{D}} \tag{3.26}$$

can and will determine two different regions in k-space. In that case, since only situations with interband coupling are considered here, the union of regions in k-space determined by (3.25) and (3.26) is considered, because it is expected that the interband interaction will mix electrons from either of those between different bands. The region is denoted by S and defined as

$$\mathbf{k} \in S \implies \varepsilon_F - \hbar\omega_{\mathrm{D}} < \varepsilon_\alpha(\mathbf{k}) < \varepsilon_F + \hbar\omega_{\mathrm{D}},\ \alpha \in \{1,2\}. \tag{3.27}$$

It is expected, of course, that the width of the shells remains smaller than the Fermi vector

$$\Delta k \ll k_F. \tag{3.28}$$

Figure 3.4 depicts the region of k-space (highlighted) to which the interaction is confined for a given $\mathbf{K}$-vector. The different possibilities for the choice of this vector depending on the band structure is the main difference between the next three chapters.

3.3.2 Intraband Coupling

Interaction between electrons in the same bands is considered here. This includes the case where both of them change the band (so the potentials V_{11}^{11}, V_{22}^{22}, V_{11}^{22} and V_{22}^{11}). In those cases, in figure 3.4 $k_{\mathrm{F1}} = k_{\mathrm{F2}}$ and the process is most effective when $\mathbf{K} = 0$ and in turn only those are looked at. This is exactly the same approximation also made in BCS theory.

Furthermore, since the shells are narrow, the potentials are taken to be constant in it and zero otherwise. This means that the interaction constants are approximated as follows

$$V_{\alpha\alpha}^{\beta\beta}(\mathbf{K},\mathbf{k},\mathbf{q}) = \begin{cases} V_{\alpha\alpha}^{\beta\beta}\delta_{\mathbf{K},0} & \mathbf{k},\mathbf{k}+\mathbf{q}\in S \\ 0 & \text{otherwise} \end{cases}, \tag{3.29}$$

$$V_{11}^{11} = -\frac{|G_{11}|^2}{\hbar\overline{\omega}_{11}}, \tag{3.30}$$

$$V_{22}^{22} = -\frac{|G_{22}|^2}{\hbar\overline{\omega}_{22}}, \tag{3.31}$$

$$V_{11}^{22} = V_{22}^{11*} = -\frac{(G_{12})^2}{\hbar\overline{\omega}_{12}}. \tag{3.32}$$

The $\overline{\omega}$ represent average or characteristic phonon frequency and $G_{\alpha\beta}$ are likewise electron-phonon interaction constants which either are independent of $\mathbf{q}$ and $\mathbf{k}$ (for s-waves) or are averaged over the indices.

It should be noted that although V_{11}^{11} and V_{22}^{22} turn out to be real and negative (as required by one-band BCS theory), $V_{11}^{22} = V_{22}^{11*}$ can be a general complex number (just like $G_{12} = G_{21}^{*}$). Those potentials are real if G_{12} is either real or purely imaginary: in the first case $V_{11}^{22} = V_{22}^{11} < 0$ and in the second case $V_{11}^{22} = V_{22}^{11} > 0$. It has been shown [34] that either of those cases will give a stable superconducting state. This also shows that even purely interband electron-phonon coupling can lead to intraband pairing of electrons.

3.3.3 Interband Non-FFLO Coupling

The interband electron-electron interaction is now considered. Included are also the cases where only one electron changes the band. The most similar situation to BCS theory of superconductivity is when the Fermi surfaces of the two bands overlap so that in our case $k_{\mathrm{F1}} \approx k_{\mathrm{F2}}$ (in fact, equality is assumed). It does not mean that $\varepsilon_1(\mathbf{k}) = \varepsilon_2(\mathbf{k})$ just that they

intersect in the Fermi level. In a model with parabolic dispersion relations, this can be achieved with a constant term (shifting of the Fermi level) for one of the bands.

The situation is the same as in the intraband case in figure 3.4. The most effective processes (the rest are assumed to average out similarly to chaotic phase cancellation) are for $\mathbf{K} = 0$. This is in contrast to the next section where the condition $\mathbf{K} = \pm\mathbf{Q} \neq 0$ implies a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [35, 36]. The current case is termed non-FFLO coupling and gives interband Cooper pairs with zero net momentum.

The non-FFLO interband potentials are approximated just like intraband ones (cf. (3.29) which is actually included here).

$$V_{\alpha_1\alpha_2}^{\alpha_1'\alpha_2'}(\mathbf{K},\mathbf{k},\mathbf{q}) = \begin{cases} V_{\alpha_1\alpha_2}^{\alpha_1'\alpha_2'}\delta_{\mathbf{K},0} & \mathbf{k},\mathbf{k}+\mathbf{q}\in S \\ 0 & \text{otherwise} \end{cases}, \tag{3.33}$$

$$V_{12}^{21} = V_{21}^{12} = -\frac{|G_{12}|^2}{\hbar\overline{\omega}_{12}}, \tag{3.34}$$

$$V_{12}^{12} = V_{21}^{21} = -\frac{G_{22}G_{11}}{2\hbar\left(\overline{\omega}_{11}^{-1}+\overline{\omega}_{22}^{-1}\right)^{-1}}, \tag{3.35}$$

$$V_{11}^{12} = V_{11}^{21} = V_{21}^{11*} = V_{12}^{11*} = -\frac{G_{12}G_{11}}{2\hbar\left(\overline{\omega}_{11}^{-1}+\overline{\omega}_{12}^{-1}\right)^{-1}}, \tag{3.36}$$

$$V_{21}^{22} = V_{12}^{22} = V_{22}^{12*} = V_{22}^{21*} = -\frac{G_{12}G_{22}}{2\hbar\left(\overline{\omega}_{22}^{-1}+\overline{\omega}_{12}^{-1}\right)^{-1}}. \tag{3.37}$$

As was the case with interband electron-phonon interaction giving rise to intraband pairing, so can purely intraband electron-phonon interaction give rise to interband pairing.

$V_{12}^{21} = V_{21}^{12}$ is always negative, but $V_{12}^{12} = V_{21}^{21}$ can be either positive or negative (but real) depending on whether G_{11} and G_{22} have the same or opposite sign. The potentials (3.36) and (3.37) are in general complex with the same or opposite phase as G_{12}.

3.3.4 Interband FFLO Coupling

In this section an alternative to the previous interband approximation is proposed. In general the Fermi surfaces do not overlap so $|k_{\mathrm{F}1} - k_{\mathrm{F}2}| \gg \hbar\omega_{\mathrm{D}}$. As per figure (3.4), this means that $\mathbf{K} = 0$ terms should disappear. It is then possible that, as in the previous section (3.3.3), the interband terms don't give measurable effects. Another possibility is that the $\mathbf{K}$-vector is allowed to take two values $\pm\mathbf{Q}$. This corresponds to FFLO superconducting state, which is usually connected to magnetic splitting of spin up and down states (one can then consider them as up and down „bands“) [35, 36, 37]. In the context of electron-phonon interaction, this splitting comes from the existence of two different bands without

an external magnetic field.

The FFLO state is characterized by a non-uniform order parameter (or superconducting gap, defined in the next sections)

$$\Delta(\mathbf{r}) = \Delta_{\mathbf{Q}} e^{i\mathbf{Q}\cdot\mathbf{r}}. \tag{3.38}$$

It is proposed in [38] that even when $\mathbf{Q}$ is not actually restricted to a single axis, the order parameter in this case can be written as

$$\Delta(\mathbf{r}) = \sum_{\mathbf{Q}} \Delta_{\mathbf{Q}} e^{i\mathbf{Q}\cdot\mathbf{r}}, \tag{3.39}$$

where the sum is over all the considered $\mathbf{Q}$-vectors (all vectors on a sphere in an isotropic case).

The interband interaction potentials for the FFLO case can be approximated as[6]

$$V_{\alpha\overline{\alpha}}^{\beta\overline{\beta}}(\mathbf{K},\mathbf{k},\mathbf{q}) = \begin{cases} V_{\alpha\overline{\alpha}}^{\beta\overline{\beta}}\left(\delta_{\mathbf{K},\mathbf{Q}} + \delta_{\mathbf{K},-\mathbf{Q}}\right) & \mathbf{K}+\mathbf{k},\, \mathbf{K}+\mathbf{k}+\mathbf{q} \in S \\ 0 & \text{otherwise} \end{cases}, \tag{3.40}$$

$$V_{12}^{21} = V_{21}^{12} = -\frac{|G_{12}|^2}{\hbar\overline{\omega}_{12}}, \tag{3.41}$$

$$V_{12}^{12} = V_{21}^{21} = -\frac{G_{22}G_{11}}{2\hbar\left(\overline{\omega}_{11}^{-1} + \overline{\omega}_{22}^{-1}\right)^{-1}}, \tag{3.42}$$

The processes where only one electron changes the band violates momentum conservation and is thus zero.

A reasonable choice for $|\mathbf{Q}|$, according to figure 3.4 and the argument that the interaction volume in k-space should be maximal, is $|\mathbf{Q}| = \sqrt{\left|k_{\mathrm{F1}}^2 - k_{\mathrm{F2}}^2\right|}$.This means that when $k_{\mathrm{F1}} > k_{\mathrm{F2}}$, the electron belonging to the second band has a momentum that is nearly perpendicular to $\mathbf{Q}$. So the integration volume in k-space consists of two rings (with cross-section $\sim (\Delta k)^2$ where Δk is the shift in k-space corresponding to energy shift $2\hbar\omega_{\mathrm{D}}$) of radius k_{F2}centered on $\pm\mathbf{Q}$ and perpendicular to $\mathbf{Q}$. This is different from the situations in two previous sections, where the integration volume was just a shell around the Fermi sphere. In particular, the integration can not be carried out in ε- space for the FFLO case.

[6]Here and below for band indices (as with spin indices) $\overline{1} = 2$ and $\overline{2} = 1$ is used for convenience as it allows to write out general interband terms (for two bands) without additional conditions.

4 The Superconductive (Non-FFLO) Hamiltonian

A quick overview of this section: using the potentials from sections 3.3.3 and 3.3.4, the mean-field approximation is applied to the Hamiltonian (3.17) through which the order parameters (gaps) associated with superconductivity (which have the form $\Delta = \sum \langle aa \rangle$) are introduced. A Bogolyubov transformation is performed replacing the a operators with γ operators (Fermi creation-annihilation operators for elementary exitations of the system) in which the mean-field Hamiltonian is diagonal. These are substituted into the gaps' definitions so $\Delta = \sum \langle \gamma^\dagger \gamma \rangle = \sum f(E)$ where $f(E)$ is the Fermi distribution, which gives a system of equations for the order parameters (the gap equations).

4.1 Mean-field Approximation

A mean-field approximation is of the form

$$H^A H^B = H^{AB}_{MF} \approx H^A \langle H^B \rangle + \left\langle H^A \right\rangle H^B - \left\langle H^A \right\rangle \langle H^B \rangle$$

and essentially means that the average effect of system A on system B is $H^A \langle H^B \rangle$ and vice versa. The $\left\langle H^A \right\rangle \langle H^B \rangle$ terms make sure that $\langle H^A H^B \rangle = \langle H^{AB}_{MF} \rangle$. This kind of factorization is often quite difficult (and describes different effects) and relies on intuition and the averages actually existing. Superconductivity in one band is associated with the so-called anomalous averages $\langle a_{\mathbf{k}\sigma} a_{-\mathbf{k}\overline{\sigma}} \rangle$. The generalization for two bands is straightforward.

The Hamiltonian (3.17) with potentials from sections 3.3.3 and 3.3.4 (taking into account the remarks in the beginning of section 3.3 regarding spin and phonon indices) is

$$\begin{aligned} H &= \sum_{\alpha,\mathbf{k},\sigma} \left[\varepsilon_\alpha(\mathbf{k}) - \varepsilon_F\right] a^\dagger_{\mathbf{k}\alpha\sigma} a_{\mathbf{k}\alpha\sigma} \\ &+ \sum_{\alpha_1,\alpha_2,\alpha_1',\alpha_2'} V^{\alpha_1'\alpha_2'}_{\alpha_1\alpha_2} \sum_{(\mathbf{k},\mathbf{k}+\mathbf{q}\in S),\sigma} a^\dagger_{\mathbf{k}+\mathbf{q},\alpha_1'\sigma} a^\dagger_{-\mathbf{k}-\mathbf{q},\alpha_2'\overline{\sigma}} a_{-\mathbf{k}\alpha_2\overline{\sigma}} a_{\mathbf{k}\alpha_1\sigma}, \end{aligned} \tag{4.1}$$

where S denotes region of k-space where the interaction constant is non-zero, which is taken to be the same in both bands for simplicity.

The interaction constants have the following symmetries.

$$V^{\alpha_1'\alpha_2'}_{\alpha_1\alpha_2} = V^{\alpha_1\alpha_2 *}_{\alpha_1'\alpha_2'} \tag{4.2}$$

$$V^{\alpha_1'\alpha_2'}_{\alpha_1\alpha_2} = V^{\alpha_2'\alpha_1'}_{\alpha_2\alpha_1} \tag{4.3}$$

Applying the mean-field approximation yields, after some rearrangement

$$\begin{aligned} H_{\mathrm{mf}} &= H_{\mathrm{const}} + \sum_{\alpha,\mathbf{k},\sigma} \left[\varepsilon_\alpha(\mathbf{k}) - \varepsilon_F\right] a^\dagger_{\mathbf{k}\alpha\sigma} a_{\mathbf{k}\alpha\sigma} \\ &+ \sum_{\alpha_1,\alpha_2} \sum_{\mathbf{k}\in S,\sigma} \left[\Delta^{\sigma\overline{\sigma}*}_{\alpha_1\alpha_2} a_{-\mathbf{k}\alpha_2\overline{\sigma}} a_{\mathbf{k}\alpha_1\sigma} + \Delta^{\sigma\overline{\sigma}}_{\alpha_1\alpha_2} a^\dagger_{\mathbf{k}\alpha_1\sigma} a^\dagger_{-\mathbf{k}\alpha_2\overline{\sigma}}\right], \qquad (4.4) \\ \Delta^{\sigma\overline{\sigma}*}_{\alpha_1\alpha_2} &= \sum_{\alpha_1',\alpha_2'} \sum_{\mathbf{k}\in S} V^{\alpha_1'\alpha_2'}_{\alpha_1\alpha_2} \left\langle a^\dagger_{\mathbf{k}\alpha_1'\sigma} a^\dagger_{-\mathbf{k}\alpha_2'\overline{\sigma}} \right\rangle. \qquad (4.5) \end{aligned}$$

The expressions under the sums are obviously Hermitian. The order parameter $\Delta^{\sigma\overline{\sigma}*}_{\alpha_1\alpha_2}$ [7] has the following symmetry from Fermi commutation rules.

$$\Delta^{\sigma\overline{\sigma}}_{\alpha_1\alpha_2} = -\Delta^{\overline{\sigma}\sigma}_{\alpha_2\alpha_1} \qquad (4.6)$$

The intraband case $\Delta^{\uparrow\downarrow}_{\alpha\alpha} = -\Delta^{\downarrow\uparrow}_{\alpha\alpha}$ can be attributed to the antisymmetricity of the spin part of the wavefunction. The interband case implies that the spin part doesn't need to be antisymmetric if the band part is and vice versa.

4.2 Diagonalization

4.2.1 Bogolyubov Transformations

A general Hamiltonian consisting of terms up to quadratic in Fermi operators can be written as

$$\begin{aligned} H &= \sum_{\mu\nu=1}^{N} \left\{2\varepsilon_{\mu\nu} a^\dagger_\mu a_\nu + \Delta^*_{\mu\nu} a_\nu a_\mu + \Delta_{\mu\nu} a^\dagger_\mu a^\dagger_\nu\right\} \qquad (4.7) \\ &= \begin{pmatrix} A \\ A^* \end{pmatrix}^\dagger \begin{pmatrix} \varepsilon & \Delta \\ \Delta^\dagger & -\varepsilon^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} A \\ A^* \end{pmatrix} \qquad (4.8) \\ A &= \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} \qquad (4.9) \end{aligned}$$

where the coefficients can always be symmetrized with regards to Fermi anticommutation rules, which gives $\varepsilon_{\mu\nu} = \varepsilon^*_{\nu\mu}$ or $\varepsilon = \varepsilon^\dagger$, and Hermitian conjugation of the Hamiltonian, which gives $\Delta_{\mu\nu} = -\Delta_{\nu\mu}$. The vectors $\begin{pmatrix} A \\ A^* \end{pmatrix}$ is known as a Nambu vector.

It can be shown (see the thorough article [39]) that the Fermi commutation rules are

[7] The spin indices are not necessary in a single band case, because then $\Delta = \Delta^{\uparrow\downarrow} = -\Delta^{\downarrow\uparrow}$.

preserved if a unitary transformation is made like this:

$$H = \begin{pmatrix} A \\ A^* \end{pmatrix}^\dagger U^\dagger U \begin{pmatrix} \varepsilon & \Delta \\ \Delta^\dagger & -\varepsilon^{\mathrm{T}} \end{pmatrix} U^\dagger U \begin{pmatrix} A \\ A^* \end{pmatrix} \tag{4.10}$$

$$= \begin{pmatrix} B \\ B^* \end{pmatrix}^\dagger U \begin{pmatrix} \varepsilon & \Delta \\ \Delta^\dagger & -\varepsilon^{\mathrm{T}} \end{pmatrix} U^\dagger \begin{pmatrix} B \\ B^* \end{pmatrix}. \tag{4.11}$$

The $2N$ order unitary matrix of the form $\begin{pmatrix} U & V \\ V^* & U^* \end{pmatrix}$ is chosen as to diagonalize the Hamiltonian in the new operators. This is known as a Bogolyubov transformation. This gives an illustration that the diagonalization of the Hamiltonian (4.4) can be thought of as diagonalizing a matrix when it is written with Nambu vectors.

Now, in general one would have to solve for the eigenvalues and -vectors of the matrix $\begin{pmatrix} \varepsilon & \Delta \\ \Delta^\dagger & -\varepsilon^{\mathrm{T}} \end{pmatrix}$. But the problem is made immensely easier, if this matrix can be made block-diagonal with a certain order of operators in the Nambu vectors. Then we would have a sum

$$H = \sum_j \begin{pmatrix} A_j \\ A_j^* \end{pmatrix}^\dagger \begin{pmatrix} \varepsilon_j & \Delta_j \\ \Delta_j^\dagger & -\varepsilon_j^{\mathrm{T}} \end{pmatrix} \begin{pmatrix} A_j \\ A_j^* \end{pmatrix}_j,$$

where the index j labels the different blocks. The transformation can now be made inside these blocks separately (it is important that all the $\begin{pmatrix} A_j \\ A_j^* \end{pmatrix}$ contain *different* operators, otherwise it wouldn't really be block-diagonal). In the language of sums of operators it means that if and whenever the Hamiltonian (4.7) can be written as a sum of terms which don't share operators with the same quantum numbers, the terms can be diagonalized with a Bogolyubov transformation *separately*. The importance of this cannot be understated. For the Hamiltonian (4.4) it reduces the problem of diagonalizing a $2N$x$2N$ matrix to diagonalizing $\frac{N}{2}$ 4x4 matrices. This is the reason for the seemingly brutal simplification made in section 3.3 regarding the **K**-vector – it wouldn't be analytically solvable (and possibly not even numerically).

4.2.2 Bogolyubov Transformation of the Mean-field Hamiltonian

As per the last section the Hamiltonian (4.4) can be written as

$$H_{mf} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^{\dagger} H_{\mathbf{k}} \Psi_{\mathbf{k}} + H'_{\text{const}}, \tag{4.12}$$

$$H_{\mathbf{k}\in S} = \begin{bmatrix} \tilde{\varepsilon}_1(\mathbf{k}) & 0 & \Delta_{11} & \Delta_{12} \\ 0 & \tilde{\varepsilon}_2(\mathbf{k}) & \Delta_{21} & \Delta_{22} \\ \Delta_{11}^* & \Delta_{21}^* & -\tilde{\varepsilon}_1(\mathbf{k}) & 0 \\ \Delta_{12}^* & \Delta_{22}^* & 0 & -\tilde{\varepsilon}_2(\mathbf{k}) \end{bmatrix}, \tag{4.13}$$

$$H_{\mathbf{k}\notin S} = \begin{bmatrix} \tilde{\varepsilon}_1(\mathbf{k}) & 0 & 0 & 0 \\ 0 & \tilde{\varepsilon}_2(\mathbf{k}) & 0 & 0 \\ 0 & 0 & -\tilde{\varepsilon}_1(\mathbf{k}) & 0 \\ 0 & 0 & 0 & -\tilde{\varepsilon}_2(\mathbf{k}) \end{bmatrix}, \tag{4.14}$$

$$\Psi_{\mathbf{k}}^{\dagger} = \begin{bmatrix} a_{\mathbf{k}1\uparrow}^{\dagger} & a_{\mathbf{k}2\uparrow}^{\dagger} & a_{-\mathbf{k}1\downarrow} & a_{-\mathbf{k}2\downarrow} \end{bmatrix}, \tag{4.15}$$

$$\Delta_{\alpha\beta} = 2\Delta_{\alpha\beta}^{\uparrow\downarrow}. \tag{4.16}$$

This construction guarantees that no two terms of 4.12 involve the same electron creation (or annihilation) operator. Which means the Bogolyubov transformation can be applied separately to those terms. The unitary transformation must diagonalize the matrix $H_{\mathbf{k}}$:

$$U_{\mathbf{k}} H_{\mathbf{k}} U_{\mathbf{k}}^{\dagger} = \begin{bmatrix} E_{1\uparrow}(\mathbf{k}) & 0 & 0 & 0 \\ 0 & E_{2\uparrow}(\mathbf{k}) & 0 & 0 \\ 0 & 0 & -E_{1\downarrow}(\mathbf{k}) & 0 \\ 0 & 0 & 0 & -E_{2\downarrow}(\mathbf{k}) \end{bmatrix} = E_{\mathbf{k}}, \tag{4.17}$$

$$U_{\mathbf{k}} U_{\mathbf{k}}^{\dagger} = I_4 \tag{4.18}$$

$$U_{\mathbf{k}\notin S} = I_4 \tag{4.19}$$

where the diagonal entries are the eigenvalues of $H_{\mathbf{k}}$ (real because $H_{\mathbf{k}}$ is Hermitian) determined by the characteristic equation

$$0 = \det\left(H_{\mathbf{k}} - E(\mathbf{k}) \cdot I_4\right) \tag{4.20}$$

$$\begin{aligned} &= E(\mathbf{k})^4 - \left(\tilde{\varepsilon}_1(\mathbf{k})^2 + \tilde{\varepsilon}_2(\mathbf{k})^2 + |\Delta_{11}|^2 + |\Delta_{12}|^2 + |\Delta_{21}|^2 + |\Delta_{22}|^2\right) E(\mathbf{k})^2 \\ &+ \left(\tilde{\varepsilon}_2(\mathbf{k}) - \tilde{\varepsilon}_1(\mathbf{k})\right)\left(|\Delta_{12}|^2 - |\Delta_{21}|^2\right) E(\mathbf{k}) \\ &+ |\Delta_{11}\Delta_{22} - \Delta_{12}\Delta_{21}|^2 + \tilde{\varepsilon}_1(\mathbf{k})^2 \tilde{\varepsilon}_2(\mathbf{k})^2 + \tilde{\varepsilon}_1(\mathbf{k})\tilde{\varepsilon}_2(\mathbf{k})\left(|\Delta_{12}|^2 + |\Delta_{21}|^2\right). \end{aligned} \tag{4.21}$$

Since $H_{\mathbf{k}} = H_{-\mathbf{k}}$ then also $U_{\mathbf{k}} = U_{-\mathbf{k}}$ and $E(\mathbf{k}) = E(-\mathbf{k})$.

The columns of $U_{\mathbf{k}}^{\dagger}$ are eigenvectors of $H_{\mathbf{k}}$ corresponding to the eigenvalues in (4.17). Unitarity is enforced by normalizing them to one (they are orthogonal because $H_{\mathbf{k}}$ is Hermitian). The transformation is parametrized as

$$U_{\mathbf{k}} = \begin{bmatrix} u_{\mathbf{k}\uparrow}(1,1) & u_{\mathbf{k}\uparrow}(1,2) & v^*_{\mathbf{k}\downarrow}(1,1) & v^*_{\mathbf{k}\downarrow}(1,2) \\ u_{\mathbf{k}\uparrow}(2,1) & u_{\mathbf{k}\uparrow}(2,2) & v^*_{\mathbf{k}\downarrow}(2,1) & v^*_{\mathbf{k}\downarrow}(2,2) \\ v_{\mathbf{k}\uparrow}(1,1) & v_{\mathbf{k}\uparrow}(1,2) & u^*_{\mathbf{k}\downarrow}(1,1) & u^*_{\mathbf{k}\downarrow}(1,2) \\ v_{\mathbf{k}\uparrow}(2,1) & v_{\mathbf{k}\uparrow}(2,2) & u^*_{\mathbf{k}\downarrow}(2,1) & u^*_{\mathbf{k}\downarrow}(2,2) \end{bmatrix}. \tag{4.22}$$

The parametrization is justified because equation (4.20) with spin indices changed gives opposite eigenvalues.[8] It also guarantees that the transformed (quasiparticle) operators can be parametrized just like the old ones.

$$\tilde{\Psi}_{\mathbf{k}} = U_{\mathbf{k}}\Psi_{\mathbf{k}} = \begin{bmatrix} \gamma_{\mathbf{k}1\uparrow} \\ \gamma_{\mathbf{k}2\uparrow} \\ \gamma^{\dagger}_{-\mathbf{k}1\downarrow} \\ \gamma^{\dagger}_{-\mathbf{k}2\downarrow} \end{bmatrix} \tag{4.24}$$

The solutions can be picked such that

$$\lim_{\text{all}\,\Delta\to 0} \begin{bmatrix} E_{1\uparrow}(\mathbf{k}) & 0 & 0 & 0 \\ 0 & E_{2\uparrow}(\mathbf{k}) & 0 & 0 \\ 0 & 0 & -E_{1\downarrow}(\mathbf{k}) & 0 \\ 0 & 0 & 0 & -E_{2\downarrow}(\mathbf{k}) \end{bmatrix} = \begin{bmatrix} \tilde{\varepsilon}_1(\mathbf{k}) & 0 & 0 & 0 \\ 0 & \tilde{\varepsilon}_2(\mathbf{k}) & 0 & 0 \\ 0 & 0 & -\tilde{\varepsilon}_1(\mathbf{k}) & 0 \\ 0 & 0 & 0 & -\tilde{\varepsilon}_2(\mathbf{k}) \end{bmatrix}. \tag{4.25}$$

this guarantees that the transformation will be an identity transformation for $\mathbf{k} \notin S$. This is not really very necessary, because it amounts to changing of the indices of a.

The transformed Hamiltonian is

$$H_{mf} = \sum_{\mathbf{k}} \Psi^{\dagger}_{\mathbf{k}} E_{\mathbf{k}} \Psi_{\mathbf{k}} + H_{\text{const}} = \sum_{\mathbf{k},\alpha,\sigma} E_{\alpha\sigma}(\mathbf{k})\, \gamma^{\dagger}_{\mathbf{k}\alpha\sigma}\gamma_{\mathbf{k}\alpha\sigma} + H_{\text{const}}, \tag{4.26}$$

$$\gamma_{\mathbf{k}\alpha\sigma} = \sum_{\beta} \left[u_{\mathbf{k}\sigma}(\alpha,\beta)\, a_{\mathbf{k}\beta\sigma} + v^*_{\mathbf{k}\overline{\sigma}}(\alpha,\beta)\, a^{\dagger}_{-\mathbf{k}\beta\overline{\sigma}} \right], \tag{4.27}$$

$$a_{\mathbf{k}\alpha\sigma} = \sum_{\beta} \left[u^*_{\mathbf{k}\sigma}(\beta,\alpha)\, \gamma_{\mathbf{k}\beta\sigma} + v^*_{\mathbf{k}\sigma}(\beta,\alpha)\, \gamma^{\dagger}_{-\mathbf{k}\beta\overline{\sigma}} \right]. \tag{4.28}$$

[8] In fact it can be shown that

$$E^{\uparrow\downarrow}_{\mathbf{k}} = \begin{bmatrix} E_1 & 0 & 0 & 0 \\ 0 & E_2 & 0 & 0 \\ 0 & 0 & E_3 & 0 \\ 0 & 0 & 0 & E_4 \end{bmatrix} \implies E^{\downarrow\uparrow}_{\mathbf{k}} = \begin{bmatrix} -E_3 & 0 & 0 & 0 \\ 0 & -E_4 & 0 & 0 \\ 0 & 0 & -E_1 & 0 \\ 0 & 0 & 0 & -E_2 \end{bmatrix}. \tag{4.23}$$

And naturally the γ-operators satisfy the Fermi commutation rules. This means that the averages over H_{mf} are

$$\begin{aligned}
\left\langle \gamma_{\mathbf{k}_1\alpha_1\sigma_1}\gamma_{\mathbf{k}_2\alpha_2\sigma_2}\right\rangle &= 0, && (4.29)\\
\left\langle \gamma^{\dagger}_{\mathbf{k}_1\alpha_1\sigma_1}\gamma_{\mathbf{k}_2\alpha_2\sigma_2}\right\rangle &= \delta_{\mathbf{k}_1,\mathbf{k}_2}\delta_{\alpha_1,\alpha_2}\delta_{\sigma_1,\sigma_2}f\left(E_{\alpha\sigma}\left(\mathbf{k}\right)\right), && (4.30)\\
f\left(E\right) &= \left[\exp\left(\frac{E}{k_{\mathrm{B}}T}\right)+1\right].^{-1} && (4.31)
\end{aligned}$$

What is missing of course is the transformation $U_{\mathbf{k}}$ itself. It turns out in the next section that it is actually not necessary to calculate it fully.

4.3 Gap Equations

The order parameters (gaps) can be determined from the so-called gap equations, which are obtained by substituting the averages obtained with (4.28) into (4.5) and taking into account (4.29) and (4.30).

$$\begin{aligned}
\left\langle a_{-\mathbf{k}\alpha_2\downarrow}a_{\mathbf{k}\alpha_1\uparrow}\right\rangle &= \sum_{\beta}u^{*}_{\mathbf{k}\downarrow}\left(\beta,\alpha_2\right)v^{*}_{\mathbf{k}\uparrow}\left(\beta,\alpha_1\right)f\left(-E_{\beta\downarrow}\left(\mathbf{k}\right)\right)\\
&+ \sum_{\beta}u^{*}_{\mathbf{k}\uparrow}\left(\beta,\alpha_1\right)v^{*}_{\mathbf{k}\downarrow}\left(\beta,\alpha_2\right)f\left(E_{\beta\uparrow}\left(\mathbf{k}\right)\right) \qquad (4.32)
\end{aligned}$$

$$\begin{aligned}
\Delta_{\alpha_1\alpha_2} &= 2\sum_{\alpha_1',\alpha_2'}\sum_{\beta}\sum_{\mathbf{k}\in S}V^{\alpha_1\alpha_2}_{\alpha_1'\alpha_2'}\left[u^{*}_{\mathbf{k}\downarrow}\left(\beta,\alpha_2'\right)v^{*}_{\mathbf{k}\uparrow}\left(\beta,\alpha_1'\right)\left[f\left(-E_{\beta\downarrow}\left(\mathbf{k}\right)\right)\right]\right]\\
&+ 2\sum_{\alpha_1',\alpha_2'}\sum_{\beta}\sum_{\mathbf{k}\in S}V^{\alpha_1\alpha_2}_{\alpha_1'\alpha_2'}\left[u^{*}_{\mathbf{k}\uparrow}\left(\beta,\alpha_1'\right)v^{*}_{\mathbf{k}\downarrow}\left(\beta,\alpha_2'\right)f\left(E_{\beta\uparrow}\left(\mathbf{k}\right)\right)\right] \qquad (4.33)
\end{aligned}$$

The temperature dependence of the gaps is implied.

It is now taken into account that the Fermi surfaces overlap and that at least in the region S the bands are isotropic and related by

$$\tilde{\varepsilon}_2\left(\mathbf{k}\right)=\tilde{\varepsilon}_2\left(\left|\mathbf{k}\right|\right)=M\tilde{\varepsilon}_1\left(\left|\mathbf{k}\right|\right)=M\tilde{\varepsilon}_1\left(\mathbf{k}\right). \qquad (4.34)$$

This can be achieved for example in the heavy fermion model with $M=\frac{m_1}{m_2}$. Though $\varepsilon_2\left(0\right)\neq 0$ for parabolic dispersion relations. Taking $0<M<1$, the region S is determined by

$$-\hbar\omega_{\mathrm{D}}\leq\tilde{\varepsilon}_1\leq\hbar\omega_{\mathrm{D}}. \qquad (4.35)$$

The density of states ρ_{F1} is taken to be constant in this shell, which allows to go from

summation in k-space to integration in ε-space.

$$\Delta_{\alpha_1\alpha_2} = 2\rho_{F1}\sum_{\alpha_1',\alpha_2'} V_{\alpha_1'\alpha_2'}^{\alpha_1\alpha_2}\sum_{\beta}\int_{-\hbar\omega_D}^{\hbar\omega_D} \mathrm{d}\varepsilon \left[u_{\varepsilon\downarrow}^{*}\left(\beta,\alpha_2'\right) v_{\varepsilon\uparrow}^{*}\left(\beta,\alpha_1'\right)\left[f\left(-E_{\beta\downarrow}(\varepsilon)\right)\right]\right] \quad (4.36)$$

$$+ \; 2\rho_{F1}\sum_{\alpha_1',\alpha_2'} V_{\alpha_1'\alpha_2'}^{\alpha_1\alpha_2}\sum_{\beta}\int_{-\hbar\omega_D}^{\hbar\omega_D} \mathrm{d}\varepsilon \left[u_{\varepsilon\uparrow}^{*}\left(\beta,\alpha_1'\right) v_{\varepsilon\downarrow}^{*}\left(\beta,\alpha_2'\right) f\left(E_{\beta\uparrow}(\varepsilon)\right)\right], \quad (4.37)$$

$$U_\varepsilon = U_{\mathbf{k}}\big|_{\tilde{\varepsilon}_1(\mathbf{k})=\varepsilon}, \quad (4.38)$$

$$E_{\beta\sigma}(\varepsilon) = E_{\beta\sigma}(\mathbf{k})\big|_{\tilde{\varepsilon}_1(\mathbf{k})=\varepsilon}. \quad (4.39)$$

For the purposes of numerical calculations, this is cast into the following form

$$\Delta_{\alpha_1\alpha_2} = 2\rho_{F1}\int_{-\hbar\omega_D}^{\hbar\omega_D}\sum_{\alpha_1',\alpha_2'=1}^{2}\sum_{j=1}^{4} V_{\alpha_1'\alpha_2'}^{\alpha_1\alpha_2} A_{\varepsilon,j,\alpha_1'} A_{\varepsilon,j,(\alpha_2'+2)}^{*} f\left(E_{\varepsilon j}\right)\mathrm{d}\varepsilon, \quad (4.40)$$

$$H_\varepsilon = \begin{bmatrix} \varepsilon & 0 & \Delta_{11} & \Delta_{12} \\ 0 & M\varepsilon & \Delta_{21} & \Delta_{22} \\ \Delta_{11}^{*} & \Delta_{21}^{*} & -\varepsilon & 0 \\ \Delta_{12}^{*} & \Delta_{22}^{*} & 0 & -M\varepsilon \end{bmatrix}, \quad (4.41)$$

$$H_\varepsilon A_{\varepsilon j} = E_{\varepsilon j} A_{\varepsilon j}, \quad (4.42)$$

in which case the transformation and its parametrization doesn't really matter.

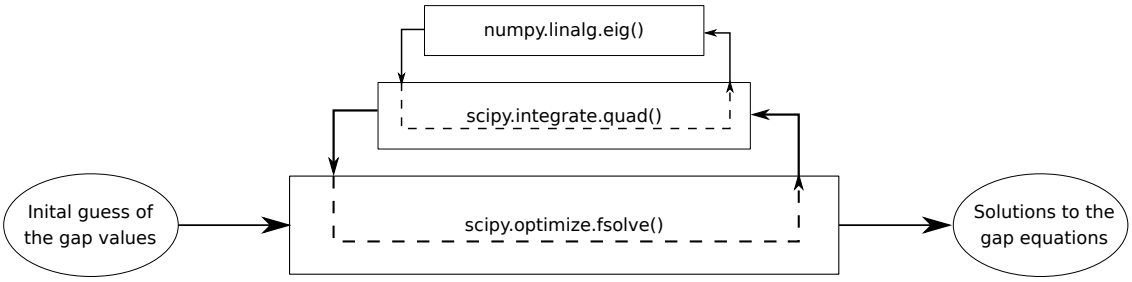


Figure 5.1: Flow chart of the numerical calculation

5 Solutions to the Gap Equations in Special Cases

Although the Hamiltonian (4.26) was derived from electron-phonon interaction, it is interesting to also look at more arbitrary cases, which cannot be explained with phonons. Specifically, limiting the possible interactions to be only between electrons of the same or different bands automatically gives either $\Delta_{12} = \Delta_{21} = 0$ or $\Delta_{11} = \Delta_{22} = 0$ respectively. This in turn allows for a reasonable analytic solution near T_C.

5.1 Numerical Calculations

In order to see the temperature-dependence of the order parameters, it is necessary to solve the gap equations numerically. To that end, algorithms from SciPy and NumPy for optimizing, integration and eigenvalue, -vector problem were used. As per chart 5.1 the calculations involved finding the roots to the gap equations which themselves include integration over a function of the gaps which in turn include finding the eigenvalues of a 4x4 matrix at each point. For consecutive temperature values, the last solution is used as a guess value. Despite the relative complexity, the equations were solved relatively quickly (about one second per solution) on a standard laptop.

The order of magnitude estimates for different parameters are:

- $\rho_{F1} \sim \frac{1}{\mathrm{eV}}$,
- $k_\mathrm{B} T_\mathrm{D} = \hbar\omega_\mathrm{D} \sim 10..100\,\mathrm{meV}$, $T_\mathrm{D} \sim 100..1000\,\mathrm{K}$, and
- $V \sim 0.1\ \mathrm{eV}$

These are of the same order as the MgB_2 parameters [40, 41]. The ratio of effective masses should be close to 1, in most of the numerical calculations it is taken as $M = 0.8$ for emphasis. The potentials and the gaps are assumed to be real, but they can be positive or negative. The gaps and $k_\mathrm{B} T_C$ should be much smaller than the Debye energy.

5.2 Only Intraband Pairing Electrons

In this section the situation where $\Delta_{12} = \Delta_{21} = 0$ is considered. To achieve this, the only interaction potentials left non-zero are V_{11}^{11}, V_{22}^{22} and $V_{11}^{22} = V_{22}^{11*}$. The numerical calculations are performed with real potentials.

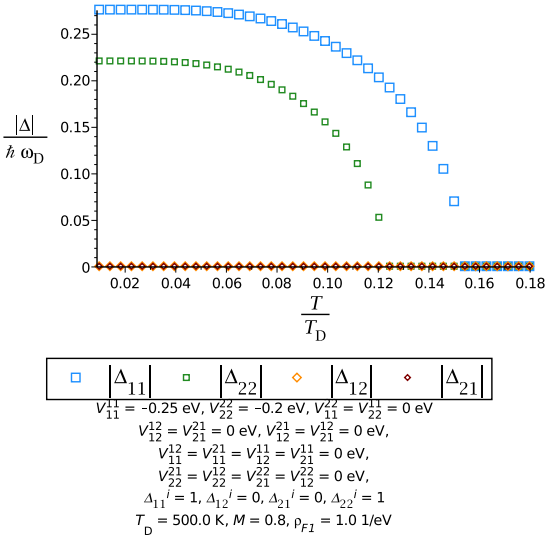
When only V_{11}^{11} is non-zero, the single band BCS gap equation is retrieved from (4.40):

$$1 = 2\rho_{F1}V_{11}^{11}\int_{-\hbar\omega_D}^{\hbar\omega_D}\frac{\tanh\left(\frac{E}{2k_BT}\right)}{\sqrt{\varepsilon^2+|\Delta|^2}}, \tag{5.1}$$

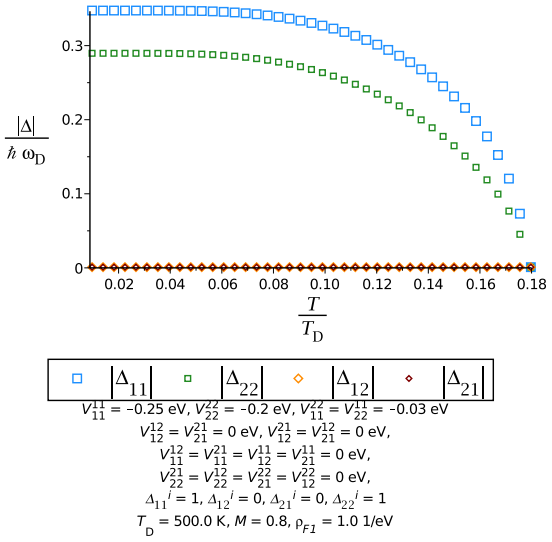
$$E = \sqrt{\varepsilon^2+|\Delta|^2}. \tag{5.2}$$

Introducing non-zero V_{22}^{22} gives just two separate BCS gap equations (modified because the shells are not the same in ε-space, $\delta\tilde{\varepsilon}_2 = M\delta\tilde{\varepsilon}_1$). When a small V_{11}^{22} (the sign does not matter) is added, the temperature dependence undergoes a qualitative change: only one critical temperature appears instead of two (compare figures 5.2a and 5.2b). This behavior is well-known [17, 42] and is not calculated analytically here.

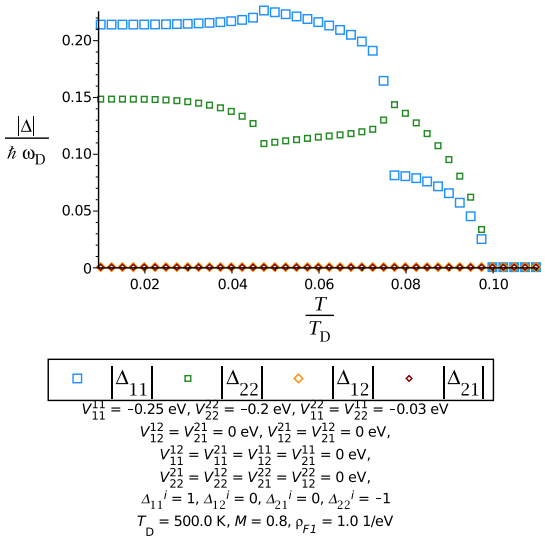
It should be noted that generally there can be many solutions to the gap equations corresponding to different relative phases between them. The different solutions indicate metastable states [43].



(a) Without pair transfer between bands



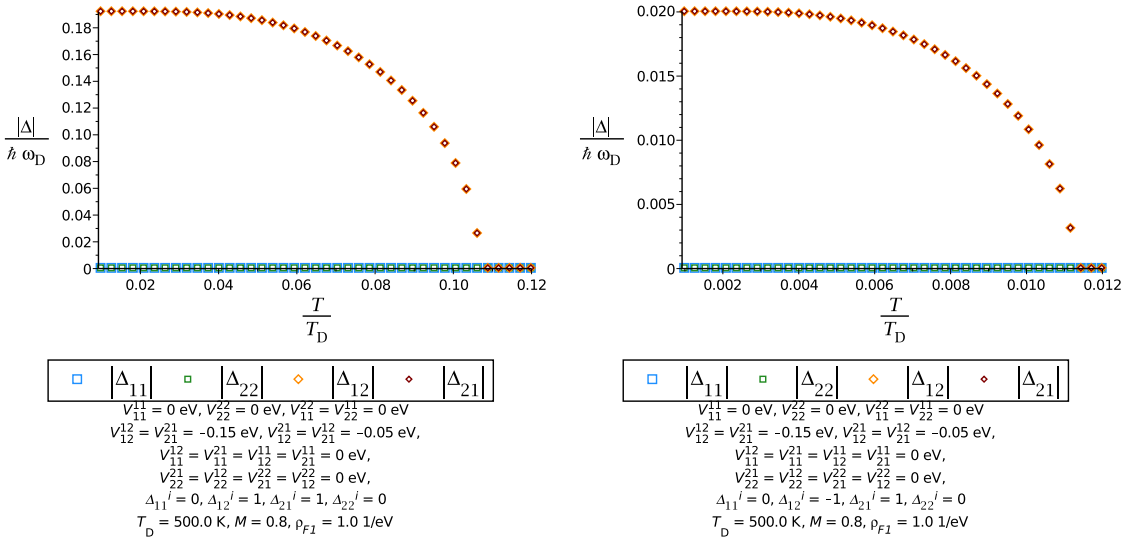
(b) With pair transfer: the even solution



(c) With pair transfer: the odd solution

Figure 5.2: Intraband el-el interaction only

5.3 Only Interband Pairing Electrons



(a) The even solution: $\Delta_{12} = \Delta_{21}$

(b) The odd solution: $\Delta_{12} = -\Delta_{21}$

Figure 5.3: Solutions to the gap equations for only interband pairing

The situation where $V_{12}^{21} = V_{21}^{12}$, $V_{12}^{12} = V_{12}^{12}$ are the only non-zero interaction potentials is considered next. The numerical calculations are shown in figures 5.3a and 5.3b. Unlike the previous case, both gaps have the same qualitative temperature dependence. The odd solution is smaller in magnitude but has a higher critical temperature than the even solution for these parameters, so it is possible for multiple solutions to the gap equations to cross as a function of temperature. [The two critical temperatures could be observable.]

Analytic solutions near T_C are sought. The gap equations for this case are

$$\Delta_{\alpha\overline{\alpha}} = 2\rho_{F1}\sum_{\beta}^{2}\sum_{j=1}^{4} V_{\beta\overline{\beta}}^{\alpha\overline{\alpha}} \int_{-\hbar\omega_D}^{\hbar\omega_D} A_{\varepsilon,j,\beta} A_{\varepsilon,j,(\overline{\beta}+2)}^{*} f\left(E_{\varepsilon j}\right) \mathrm{d}\varepsilon, \tag{5.3}$$

$$H_\varepsilon = \begin{bmatrix} \varepsilon & 0 & 0 & \Delta_{12} \\ 0 & M\varepsilon & \Delta_{21} & 0 \\ 0 & \Delta_{21}^{*} & -\varepsilon & 0 \\ \Delta_{12}^{*} & 0 & 0 & -M\varepsilon \end{bmatrix}, \tag{5.4}$$

$$H_\varepsilon A_{\varepsilon j} = E_{\varepsilon j} A_{\varepsilon j}. \tag{5.5}$$

For real interaction potentials the gaps have to be either in the same or in the opposite

phase[9]. This means that the solutions in figures 5.3a and 5.3b really are the only ones. The gap equations turn into two sets of (different) equations for the *absolute* value of the gaps

$$\Delta^{\pm}_{\alpha\overline{\alpha}} = -\Delta^{\pm}_{\alpha\overline{\alpha}} V^{12}_{12} B_{\alpha} \mp \Delta^{\pm}_{\overline{\alpha}\alpha} V^{21}_{12} B_{\overline{\alpha}}, \tag{5.10}$$

$$B_{\alpha} = \rho_{1F} \int_{-\hbar\omega_D}^{\hbar\omega_D} \mathrm{d}\varepsilon \frac{\tanh\left(\frac{E_{\varepsilon\alpha}}{2k_BT}\right) + \tanh\left(\frac{E_{\varepsilon,2+\overline{\alpha}}}{2k_BT}\right)}{\sqrt{(1+M)^2\varepsilon^2 + 4\left|\Delta_{\alpha\overline{\alpha}}\right|^2}} > 0, \tag{5.11}$$

where $\Delta^{\pm}_{\alpha\overline{\alpha}}$ are the absolute values of the even and odd solutions respectively. Linearizing the equations near $T_C^{\pm}$ (as the numerical calculations show, the order parameters approach zero together) gives the following

$$B_{\alpha}|_{T=T_C^{\pm}} = B_{\overline{\alpha}}|_{T=T_C^{\pm}} = \frac{-1}{V^{12}_{12} \pm V^{21}_{12}}, \tag{5.12}$$

from which the conditions for the existence of the solutions can be determined. This is illustrated in figure 5.4. Both solutions exist in the green region, only even or odd exist in the blue and cyan regions respectively and there are no solutions in the red region.

Analysis also shows that

$$T^{\pm} \sim \exp\left(\frac{C}{V^{12}_{12} \pm V^{21}_{12}}\right), \tag{5.13}$$

where the argument of the exponent is always negative. So $V^{21}_{12} > 0 \implies T^- > T^+$ and $V^{21}_{12} < 0 \implies T^+ > T^-$, the second situation is realized in figures 5.3. This illustrates that although attractive electron-electron interaction is generally more beneficial to

[9] Looking for eigenvectors yields

$$AD^*(E-\varepsilon)(E+M\varepsilon) = \Delta^2_{12} A^* D \tag{5.6}$$

$$BC^*(E+\varepsilon)(E-M\varepsilon) = \Delta^2_{21} B^* C \tag{5.7}$$

So the products of the eigenvectors that appear in (5.3) $A_{\varepsilon,j,1}A^*_{\varepsilon,j,4}$ and $A_{\varepsilon,j,2}A^*_{\varepsilon,j,3}$ turn out to have the same phase as the corresponding gap. The gap equations can be written

$$\Delta_{\alpha\overline{\alpha}} = \sum_{\beta} e^{i\varphi_\beta} F_\beta, \tag{5.8}$$

where $\Delta_{\alpha\overline{\alpha}} = e^{i\varphi_\alpha}\left|\Delta_{\alpha\overline{\alpha}}\right|$ and $F_\alpha \in \mathbb{R}$. So

$$\left|\Delta_{\alpha\overline{\alpha}}\right| = \sum_{\beta} e^{i(\varphi_\beta - \varphi_\alpha)} F_\beta \tag{5.9}$$

$$= F_\alpha + e^{i(\varphi_\beta - \varphi_\alpha)} F_{\overline{\alpha}}.$$

So $\varphi_{\overline{\alpha}} - \varphi_\alpha = n\pi$.

superconductivity it is not always necessary.

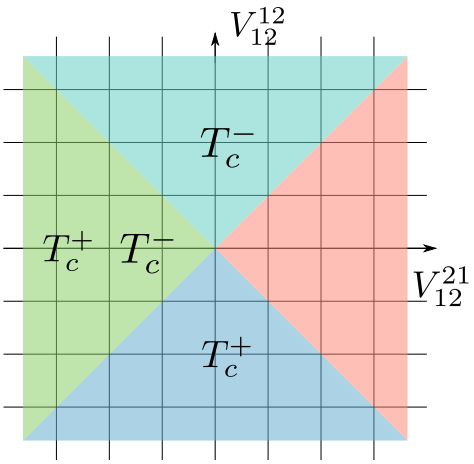


Figure 5.4: The phase diagram for the existence of even (T_C^+) or odd $\left(T_C^-\right)$ solutions

5.4 Only Intra- or Interband Electron-Phonon Interaction

Returning to the electron-phonon interaction, a few special cases are illustrated. Since now none of the equations in (4.40) disappear, the eigenvalue problem (4.42) is not block-diagonal and does not have simple solutions in general. For this reason the critical temperatures are not analytically calculated. Another difficulty is that, for four different gaps there are three phase differences which makes the gaps' temperature dependence multi-valued and potentially even complex. Because of these difficulties, only some illustrating cases are calculated numerically and possible interpretations proposed.

5.4.1 Repressed Intraband Interaction

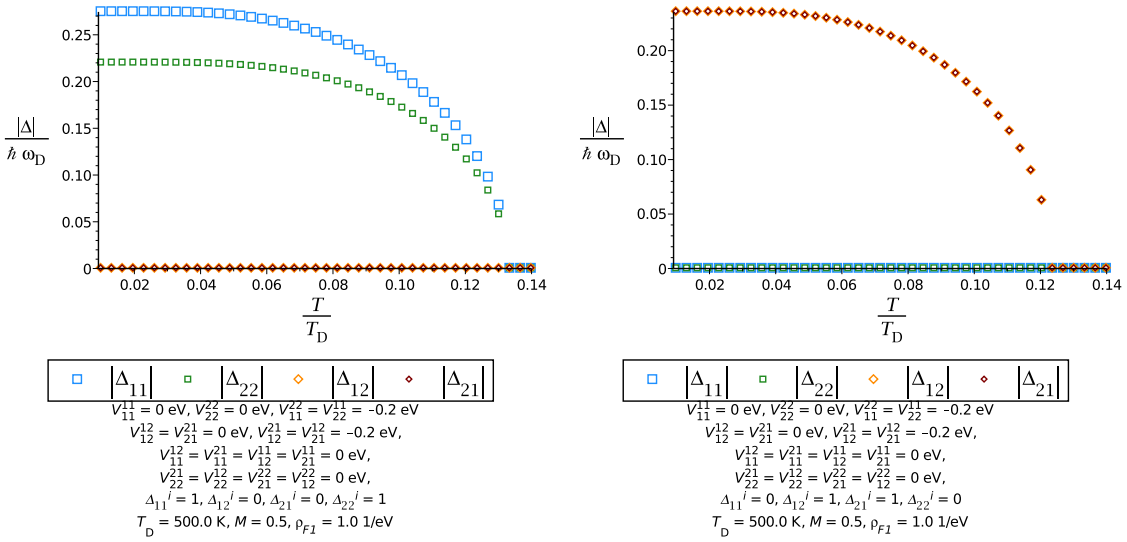
The first possibility is that the intraband electron-phonon interaction is somehow forbidden or is much smaller than the interband one. Then $G_{11} = G_{22} = 0$ and the only nonzero potentials are (3.34) and (3.32)

$$V_{12}^{21} = V_{21}^{12} = -\frac{|G_{12}|^2}{\hbar\overline{\omega}_{12}} < 0, \tag{5.14}$$

$$V_{11}^{22} = V_{22}^{11*} = -\frac{(G_{12})^2}{\hbar\overline{\omega}_{12}}. \tag{5.15}$$

To have real potentials, G_{12} has to be either real or purely imaginary in which cases $V_{11}^{22} = V_{22}^{11}$ is respectively negative or positive. Which means

$$V_{12}^{21} = V_{21}^{12} = \pm V_{11}^{22} = V_{22}^{11}. \tag{5.16}$$



(a) The intraband solution (b) The interband solution

Figure 5.5: Two solutions to intraband electron-phonon gap equations

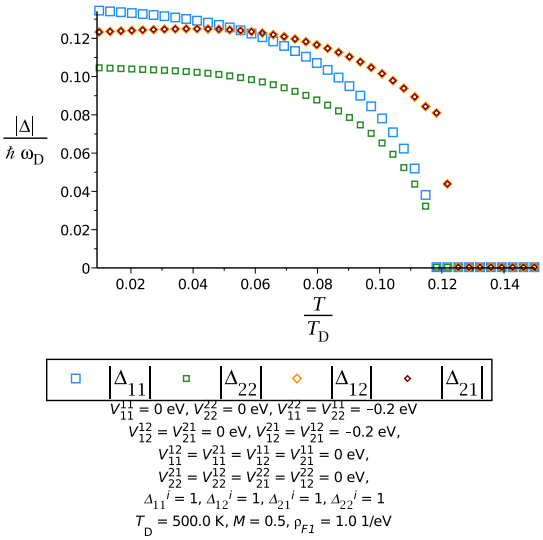


Figure 5.6: Equiphase solution

Three classes of solutions appear:

1. $\Delta_{12} = \Delta_{21} = 0$ - this solution (figure 5.5a) looks exactly like the intraband electron-electron pairing case from section 5.2. The difference of the gaps arises from M (which is lowered to 0.5 here for contrast)

2. $\Delta_{12} = \Delta_{22} = 0$ - this solution (figure (5.5b)) is analogous to the interband electron-electron pairing case from section (5.3). It corresponds to the case where $V_{12}^{12} = V_{12}^{21}$ so the solutions exist only for same-signed Δ_{12} and Δ_{21}.

3. $\operatorname{sgn}(\Delta_{11}) = \operatorname{sgn}(\Delta_{22}) = \operatorname{sgn}(\Delta_{12}) = \operatorname{sgn}(\Delta_{21})$ - all the gaps are non-zero and in the same phase (figure 5.6). This resembles the odd solution from section 5.2 (figure 5.2c). These solutions are lower in terms of both magnitude and critical temperature than the previous two solutions. The abrupt drop of $|\Delta_{12}| = |\Delta_{21}|$ is worrisome as it seems like a first-order transition (if it doesn't turn complex for example).

This behavior can also be seen from the gap equations themselves:

$$\Delta_{\alpha\alpha} = 2\rho_{F1} V_{\alpha\alpha}^{\alpha\alpha} \int_{-\hbar\omega_D}^{\hbar\omega_D} \sum_{j=1}^{4} A_{\varepsilon,j,\overline{\alpha}} A^*_{\varepsilon,j,(\overline{\alpha}+2)} f\left(E_{\varepsilon j}\right) \mathrm{d}\varepsilon, \tag{5.17}$$

$$\Delta_{\alpha\overline{\alpha}} = 2\rho_{F1} V_{\overline{\alpha}\alpha}^{\alpha\overline{\alpha}} \int_{-\hbar\omega_D}^{\hbar\omega_D} \sum_{j=1}^{4} A_{\varepsilon,j,\overline{\alpha}} A^*_{\varepsilon,j,(\alpha+2)} f\left(E_{\varepsilon j}\right) \mathrm{d}\varepsilon. \tag{5.18}$$

The solution to a situation where only V_{21}^{12} or V_{11}^{22} is non-zero is also a solution for these solutions with $\Delta_{11} = \Delta_{22} = 0$ or $\Delta_{12} = \Delta_{21} = 0$ respectively. The co-existence of both intra- and interband gaps seems less stable in this case, other methods must be employed (calculating the free energy for example) to fully answer that question.

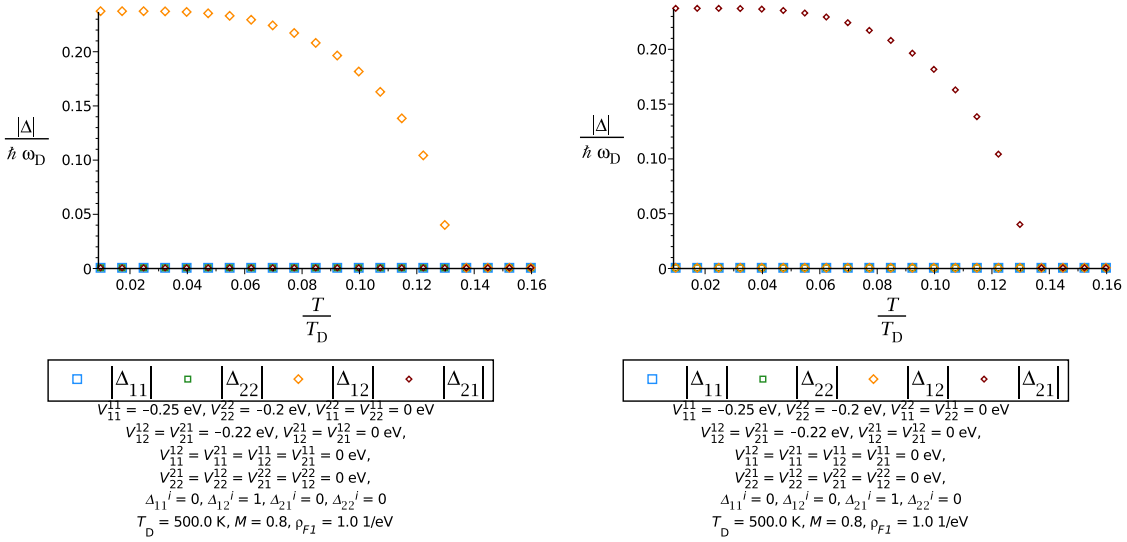
5.4.2 Repressed Interband Interaction

The second limiting case is when $G_{12} = 0$. The potentials that remain are (3.30), (3.31) and (3.35):

$$V_{11}^{11} = -\frac{|G_{11}|^2}{\hbar\overline{\omega}_{11}}, \tag{5.19}$$

$$V_{22}^{22} = -\frac{|G_{22}|^2}{\hbar\overline{\omega}_{22}}, \tag{5.20}$$

$$V_{12}^{12} = V_{21}^{21} = -\frac{G_{22}G_{11}}{2\hbar\left(\overline{\omega}_{11}^{-1} + \overline{\omega}_{22}^{-1}\right)^{-1}}, \tag{5.21}$$



(a) The isolated Δ_{12} solution

(b) The isolated Δ_{21} solution

Figure 5.7: Separate solutions for Δ_{12} and Δ_{21}

The nonzero interaction constants are V_{11}^{11}, V_{22}^{22} and $V_{12}^{12} = V_{21}^{21}$. Then

$$\Delta_{\alpha\alpha} = 2\rho_{F1} V_{\alpha\alpha}^{\alpha\alpha} \int_{-\hbar\omega_D}^{\hbar\omega_D} \sum_{j=1}^{4} A_{\varepsilon,j,\alpha} A_{\varepsilon,j,(\alpha+2)}^{*} f\left(E_{\varepsilon j}\right) \mathrm{d}\varepsilon, \tag{5.22}$$

$$\Delta_{\alpha\overline{\alpha}} = 2\rho_{F1} V_{\overline{\alpha}\alpha}^{\alpha\overline{\alpha}} \int_{-\hbar\omega_D}^{\hbar\omega_D} \sum_{j=1}^{4} A_{\varepsilon,j,\overline{\alpha}} A_{\varepsilon,j,(\alpha+2)}^{*} f\left(E_{\varepsilon j}\right) \mathrm{d}\varepsilon. \tag{5.23}$$

As in the previous case, it is expected there are decoupled solutions. But in contrast to the previous case, solutions also exist for each order parameter *individually*. What makes this really remarkable is that every other solution had $|\Delta_{12}| = |\Delta_{21}|$ and that condition is self-consistent with the gap equations[10].

[10] For certain cases it can be shown that

$$\left\langle a_{\mu\uparrow} a_{\nu\downarrow} \right\rangle = \left\langle a_{\mu\downarrow} a_{\nu\uparrow} \right\rangle \Longleftrightarrow |\Delta_{12}| = |\Delta_{21}|. \tag{5.24}$$

6 Summary

In this work, starting from a general Hamiltonian which describes interacting electron and phonon subsystems in a two-band metal, the effective electron-electron interaction constants have been derived in terms of the initial electron-phonon scattering channels and the electronic and phononic spectra. This allows to compare the efficiencies (in terms of magnitude and phase) of the different possible electron-electron interactions. An argument is made which constricts the interacting electron states to Fermi sphere, which limits the BCS-like interband pairing to materials where the bands cross at the Fermi sphere. Otherwise a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state would need to be postulated. An estimation for the most effective center of mass momentum of the FFLO electron pairs is given.

A mean-field approximation is applied to the derived Hamiltonian by postulating non-zero anomalous averages known to be related to superconductivity through which the order parameters (or gaps) are defined. This gives a Hamiltonian quadratic instead of quartic in electron creation and and annihilation operators. The Bogolyubov transformation is used to define quasiparticles in which the mean-field Hamiltonian is diagonal. Thus the elementary exitations of the system are obtained which allow one to write the anomalous averages using the Fermi distribution which together with the gap definitions give a set of coupled integral equations for determining the order parameters. Non-zero solutions to these equations indicate a possible superconducting state. The critical temperatures of systems of with only interband electron pairing are calculated and the existence of the solutions depending on the strength and phases of interaction potentials analyzed.

A script has been developed for the numerical solution of the gap equations with arbitrary parameters and special cases with realistic order of magnitude parameters calculated. A known limit of intraband pairing with pair transfer is shown to give qualitatively correct solutions. Other special cases demonstrate that the gap equations have in general several different solutions and that the phase differences between the different order parameters can be used in classifying them.

The natural extension of this work is to calculate thermodynamic quantities for real systems from the diagonal Hamiltonian and to compare the results with other known mechanisms of superconductivity. Also, the FFLO case was not thoroughly analyzed and it would be interesting to know if the Wegner's flow equations give the same result as the Fröhlich's transformation. The numerical solution could be extended to automatically search for all solutions in a given range.

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Foononite poolt vahendatav elektron-elektron interaktsioon kahetsoonilistes ülijuhtides

Heino Soo

Kokkuvõte

Käesoleva töö eesmärgiks on tuletada täielik komplekt virtuaalsete foononite poolt vahendatavaid efektiivseid elektron-elektron interaktsioonikonstante kahetsoonilise metalli jaoks, kus on arvesse võetud nii tsoonisiseseid kui ka -vahelisi foononkanaleid, ning nende kaudu ülijuhtivate korrastusparameetrite defineerimine ning leidmine.

Alustatud on üldisest kahetsoonilises metallis elektronide ja foononite (kristallvõre võnkumised) interakteeruvaid alamsüsteeme kirjeldavast hamiltoniaanist. Fröhlichi teisendust kasutades on tuletatud efektiivsed elektron-elektron interaktsioonikonstandid algsete elektron-foonon hajumiskanalite ning elektron- ja foononspektri kaudu. See võimaldab võrrelda erinevate võimalike foononite poolt vahendatavate elektron-elektron protsesside efektiivsust nii tugevuse kui faasi mõttes. On põhjendatud interakteeruvate elektronolekute Fermi sfääri lähedusse piiramine, mis pärsib oluliselt BCS-sarnast tsoonidevahelist paardumist materjalides, mille elektrontsoonid ei lõiku Fermi pinnal. Vastasel korral tuleb postuleerida Fulde-Ferrelli-Larkini-Ovchinnikovi (FFLO) olek, kus Cooperi paaridel on mingi fikseeritud nullist erinev summaarne impulss. Selle väärtust on hinnatud arvatava efektiivseima paardumise juhul.

Saadud hamiltoniaanile rakendatakse keskmise välja lähendust. Selle käigus eeldatakse n-ö anomaalsete keskmiste, mis on teadaolevalt seotud ülijuhtivusega, nullist erinevust, mille kaudu defineeritakse korrastusparameetrid (ülijuhtivuspilud): kaks tsooniseesmist ning põhimõtteliselt kaks tsoonidevahelist. Tulemuseks on hamiltoniaan, kus igas liikmes on ülimalt kaks elektronide tekkimise ja kadumise operaatorit. Bogoljubovi teisendusega defineeritakse kvaasiosakeste operaatorid, mille kaudu esitades on keskmise välja hamiltoniaan diagonaalne. Need annavad süsteemi elementaarergastused ning võimaldavad leida anomaalsed keskmised pilude funktsioonina, mis võimaldab üles kirjutada integraalvõrrandite süsteemi korrastusparameetrite määramiseks: piluvõrrandid. Nende nullist erinevad lahendid vastavad võimalikule ülijuhtivale faasile. Ainult tsoonidevahelise juhu jaoks on arvutatud ka kriitilised temperatuurid ning analüüsitud lahendite eksisteerimist sõltuvalt interaktsioonipotentsiaalide tugevustest ja faasidest.

Töö käigus arendati välja numbrilise lahendamise programm Pythoniga suvaliste parameetritega piluvõrranditele, kasutades olemasolevaid numbrilise integreerimise, optimiseerimise ja omaväärtusprobleemi lahendusmeetodeid. Oluliseimate erijuhtude jaoks on leitud pilude temperatuurne käitumine realistlike parameetrite jaoks ning saadud igal

juhul ka mittetriviaalsed lahendid. On näidatud, et piluvõrranditel on üldiselt mitu võimalikku lahendit ning et erinevate pilude faasivahe võimaldab neid klassifitseerida.

Töö loomulik edasiarendus on saadud võrrandite abil termodünaamiliste suuruste arvutamine reaalsete süsteemide jaoks ning tulemuste võrdlemine teiste ülijuhtivust esilekutsuvate mehhanismidega. Lisaks jäi põhjalikumalt vaatamata FFLO juht ning oleks huvitav teada, kas Fröhlichi teisenduse asemel Wegneri pideva teisenduse kasutamine annab sama tulemuse. Numbrilist lahendamist saaks täiendada nii, et see oleks võimeline kõik lahendid automaatselt leidma.

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